

正则长波方程的格子 Boltzmann 模型*

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摘 要 提出了用于正则长波方程的 5-Bit 格子 Boltzmann 模型。应用 Chapman-Enskog 展开和多重尺度技术, 通过选择平衡态分布函数的高阶矩, 得到了时间尺度 t_0 上的守恒律, 从而给出三阶精度的算法。模型中的参数通过稳定性分析给出。

关键词 格子 Boltzmann 方法 RLW 方程 多重尺度 5-Bit 格子 时间尺度 t_0 上的守恒律

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0 引 言

格子 Boltzmann 方法 (LBM) 用于模拟不可压缩 Navier-Stokes 方程是近几年发展起来的^[1~3]。这种方法是基于对时、空及相应宏观物理量完全离散化的数值方法, 是由格子气方法发展而来的。目前该方法已经应用到流体力学各领域。另一方面, 对于模型方程的应用是成功的。文[4]通过变换给出了 Burgers 方程的算法。对于简单的模型方程, 可以通过增加平衡态分布函数的限定条件, 适当选择平衡态的形式实现^[5,6], 在文[11]中引入 5-Bit 模型, 保留 f^3 , 适当选择时间尺度 t_0 上的守恒律, 得到了 KdV 方程的格子 Boltzmann 模型^[11]。

本文给出了截断误差是 $O(\epsilon^3)$ (ϵ 是 Knudsen 数) 的正则长波 (RLW) 方程的格子 Boltzmann 模型, 数值实验表明该方法是可行的。

此方法还可以用来构造其它非线性模型方程的格子 Boltzmann 算法, 后文将陆续给出。

1 格子 Boltzmann 模型

1.1 宏观物理量的定义

考虑一维模型, 将速度离散成 4 个方向 (如图 1), 每一个节点与相邻近的 4 个节点相连, 沿每一格线运动的粒子分布函数为 $f(x, t)$, 其中 $e = 0, 1, \dots, 4$ ($e = 0$ 表示静止粒子。为统一, 记 $b(e = 4)$ 表示格线数, $\{e\} = (0, c, -c, kc, -kc)$ 为速度集, k 是不为 0 和 1 的正数。物理量 $u(x, t)$ (粒子数) 定义为

$$u(x, t) = \sum_e f(x, t) \quad (1)$$

考虑守恒性质有

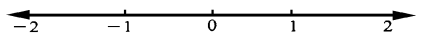


图 1 离散的格子

Fig. 1 Schematic of a 1D Lattice

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$$\sum f^{eq}(x, t) = u(x, t) \quad (2)$$

格子 Boltzmann 方程为

$$f(x + e, t + 1) - f(x, t) = - (1/\tau) [f(x, t) - f^{eq}(x, t)] \quad (3)$$

其中 $f^{eq}(x, t)$ 表示局部平衡态分布函数, τ 为弛豫时间。

1.2 多重尺度展开

我们给一个小参数 ϵ , 时间步长和 Knudsen 数均取成 ϵ^{111} , 则(3)式可以写成

$$f(x + e, t + \epsilon) - f(x, t) = - (1/\tau) [f - f^{eq}] \quad (4)$$

将(4)式左边作 Taylor 展开, 得

$$f(x + e, t + \epsilon) - f(x, t) = \sum_{n=1}^{\infty} \frac{\epsilon^n}{n!} \left[\frac{\partial}{\partial t} + e \frac{\partial}{\partial x} \right]^n f(x, t) \quad (5)$$

展到 ϵ^4 , (5)式右边

$$\begin{aligned} & \left[\frac{\partial}{\partial t} + e \frac{\partial}{\partial x} \right] f + \frac{1}{2} \left[\frac{\partial}{\partial t} + e \frac{\partial}{\partial x} \right]^2 f + \frac{1}{6} \left[\frac{\partial}{\partial t} + e \frac{\partial}{\partial x} \right]^3 f \\ & + \frac{1}{24} \left[\frac{\partial}{\partial t} + e \frac{\partial}{\partial x} \right]^4 f + O(\epsilon^5) \end{aligned} \quad (6)$$

应用 Chapman-Enskog 展开^[7]

$$f = \sum_{n=0}^{\infty} \epsilon^n f^{(n)} = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \epsilon^3 f^{(3)} + \epsilon^4 f^{(4)} + \dots, \quad (7)$$

这里记 $f^{(0)}$ 为 f^{eq} 。给出 4 个时间尺度

$$t_0 = t, \quad t_1 = \epsilon t, \quad t_2 = \epsilon^2 t, \quad t_3 = \epsilon^3 t$$

有

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \epsilon^3 \frac{\partial}{\partial t_3} + O(\epsilon^4) \quad (8)$$

由 $\epsilon^i, i=1, 2, 3, 4$ 的系数相等, 有

$$\frac{\partial f^{(0)}}{\partial t_0} + \epsilon \frac{\partial f^{(0)}}{\partial x} = - \frac{1}{\tau} f^{(1)} \quad (9)$$

$$\frac{\partial f^{(0)}}{\partial t_1} - \left(1 - \frac{1}{2}\right) \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} = - \frac{1}{\tau} f^{(2)} \quad (10)$$

$$\frac{\partial f^{(0)}}{\partial t_2} + (1 - 2) \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right) \frac{\partial f^{(0)}}{\partial t_1} + \left(2 - \frac{1}{6}\right) \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^3 f^{(0)} = - \frac{1}{\tau} f^{(3)} \quad (11)$$

$$\begin{aligned} & \frac{\partial f^{(0)}}{\partial t_3} + \left(2^2 - \frac{5}{2} + \frac{1}{2}\right) \frac{\partial}{\partial t_1} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} + (1 - 2) \frac{\partial}{\partial t_2} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right) f^{(0)} \\ & + \left(-3 + \frac{3}{2} - \frac{7}{12} + \frac{1}{24}\right) \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^4 f^{(0)} + \frac{\partial f^{(2)}}{\partial t_1} + \frac{1}{2} \frac{\partial^2 f^{(2)}}{\partial t_1^2} = - \frac{1}{\tau} f^{(4)} \end{aligned} \quad (12)$$

上面方程(9)~(12)式的详细推导过程见文[11]。

1.3 BLW 方程^[9]

对(9)~(12)式求和可以得到方程组

$$\frac{\partial u}{\partial t_0} + \frac{\partial m^0}{\partial x} = 0 \tag{13}$$

$$\frac{\partial u}{\partial t_1} + \left(\frac{1}{2} - \right) \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} = 0 \tag{14}$$

$$\frac{\partial u}{\partial t_2} + \left(-^2 - + \frac{1}{6} \right) \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^3 f^{(0)} = 0 \tag{15}$$

$$\begin{aligned} \frac{\partial u}{\partial t_3} + (1 - 2) \sum \frac{\partial}{\partial t_2} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right) f^{(0)} + \left(1 - \frac{1}{2}\right) \sum \frac{\partial f^{(2)}}{\partial t_1} \\ + (2^2 - 2 + \frac{1}{4}) \sum \frac{\partial}{\partial t_1} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} \\ + \left(-^3 + \frac{3}{2}^2 - \frac{7}{12} + \frac{1}{24}\right) \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^4 f^{(0)} = 0 \end{aligned} \tag{16}$$

由(13) + (14) × + (15) × + (16) × ,得

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial m^0}{\partial x} + \left(\frac{1}{2} - \right) \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} + ^2 \mu \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^3 f^{(0)} \\ + ^3 \left[\frac{\partial u}{\partial t_2} + (1 - 2) \sum \frac{\partial}{\partial t_2} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right) f^{(0)} + \left(1 - \frac{1}{2}\right) \sum \frac{\partial f^{(2)}}{\partial t_1} \right. \\ \left. + (2^2 - 2 + \frac{1}{4}) \sum \frac{\partial}{\partial t_1} \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^2 f^{(0)} + \left(-^3 + \frac{3}{2}^2 - \frac{7}{12} + \frac{1}{24}\right) \right. \\ \left. \sum \left(\frac{\partial}{\partial t_0} + e \frac{\partial}{\partial x}\right)^4 f^{(0)} \right] = O(^4) \end{aligned} \tag{17}$$

这里 $\mu = ^2 - + 1/2$, 如选择

$$m^0 = \sum f^{(0)} e = \frac{1}{2} u^2 + u \tag{18}$$

$$^0 = \sum f^{(0)} e^2 = \frac{1}{3} u^3 + u^2 + u \tag{19}$$

$$P^0 = \sum f^{(0)} e^3 = \frac{1}{4} u^4 + u^3 + \frac{3}{2} u^2 + u + ^1 \left(\frac{1}{2} u^2 + u\right) \tag{20}$$

$$\begin{aligned} L^0 = \sum f^{(0)} e^4 = \frac{1}{5} u^5 + u^4 + 2u^3 + u^2 + u + ^1 \left(\frac{1}{3} u^3 + u^2 + u\right) \\ + ^2 \frac{1}{3} u^3 + ^3 u^3 + ^4 u \end{aligned} \tag{21}$$

则有

$$\frac{\partial u}{\partial t_0} + \frac{\partial m^0}{\partial x} = 0 \tag{22}$$

$$\frac{\partial m^0}{\partial t_0} + \frac{\partial ^0}{\partial x} = 0 \tag{23}$$

$$\frac{\partial ^0}{\partial t_0} + \frac{\partial P^0}{\partial x} = ^1 \frac{\partial}{\partial x} \left(\frac{1}{2} u^2 + u\right) \tag{24}$$

$$\frac{\partial P^0}{\partial t_0} + \frac{\partial L^0}{\partial x} = {}_2 \frac{\partial}{\partial x} \left(\frac{1}{3} u^3 \right) + {}_3 \frac{\partial}{\partial x} u^2 + {}_4 \frac{\partial}{\partial x} u \quad (25)$$

方程(22) ~ (25)称为时间尺度 t_0 上的守恒律,其在模型构造中起关键作用。恢复的动力学方程为

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} u^2 + u \right) + \frac{\partial^3}{\partial x^3} \left(\frac{1}{2} u^2 + u \right) + {}_1 \frac{\partial^4}{\partial x^4} \left(\frac{1}{3} u^3 \right) \\ + {}_2 \frac{\partial^4}{\partial x^4} u^2 + {}_3 \frac{\partial^4}{\partial x^4} u = O(\epsilon^4) \end{aligned} \quad (26)$$

从(26)式中给出 $\partial m^0 / \partial x$, 代回(26)式消去三阶导数项得如下方程

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} u^2 + u \right) - \frac{\partial^3}{\partial x^2 \partial t} u - {}_2 \frac{\partial^5}{\partial x^5} \left(\frac{1}{2} u^2 + u \right) - {}_1 \frac{\partial^6}{\partial x^6} \left(\frac{1}{3} u^3 \right) \\ - {}_2 \frac{\partial^6}{\partial x^6} u^2 - {}_3 \frac{\partial^6}{\partial x^6} u + {}_1 \frac{\partial^4}{\partial x^4} \left(\frac{1}{3} u^3 \right) + {}_2 \frac{\partial^4}{\partial x^4} u^2 + {}_3 \frac{\partial^4}{\partial x^4} u = O(\epsilon^4) \end{aligned} \quad (27)$$

其中

$$\begin{aligned} &= {}_2 \left(\epsilon^2 - \epsilon + 1/2 \right) {}_1 \\ {}_1 &= {}_3 \left[-\epsilon^3 + (3/2)\epsilon^2 - (7/12)\epsilon + (1/24) \right] (\epsilon^2 - 3\epsilon) \\ {}_2 &= {}_3 \left[-\epsilon^3 + (3/2)\epsilon^2 - (7/12)\epsilon + (1/24) \right] (\epsilon^3 - 3\epsilon) \\ {}_3 &= {}_3 \left[-\epsilon^3 + (3/2)\epsilon^2 - (7/12)\epsilon + (1/24) \right] (\epsilon^4 - 3\epsilon) \end{aligned}$$

1.4 平衡态分布函数

上节得到关于平衡态分布函数矩的表达式

$$\sum f^{(0)} = u = B_1 \quad (28)$$

$$\sum f^{(0)} e = \frac{1}{2} u^2 + u = cB_2 \quad (29)$$

$$\sum f^{(0)} e^2 = \frac{1}{3} u^3 + u^2 + u = c^2 B_3 \quad (30)$$

$$\sum f^{(0)} e^3 = \frac{1}{4} u^4 + u^3 + \frac{3}{2} u^2 + u + {}_1 \left(\frac{1}{2} u^2 + u \right) = c^3 B_4 \quad (31)$$

$$\begin{aligned} \sum f^{(0)} e^4 &= \frac{1}{5} u^5 + u^4 + 2u^2 + u + {}_1 \left(\frac{1}{3} u^3 + u^2 + u \right) \\ &+ {}_2 (1/3) u^3 + {}_3 u^3 + {}_4 u = c^4 B_5 \end{aligned} \quad (32)$$

求得平衡态分布函数为

$$f_1^{(0)} = (1/2) (k^2 B_3 - B_5 + k^2 B_2 - B_4) / (k^2 - 1) \quad (33)$$

$$f_2^{(0)} = (1/2) (k^2 B_3 - B_5 - k^2 B_2 + B_4) / (k^2 - 1) \quad (34)$$

$$f_3^{(0)} = \frac{1}{2} \left[\frac{B_5 - B_3}{k^4 - k^2} + \frac{B_4 - B_2}{k^3 - k} \right] \quad (35)$$

$$f_4^{(0)} = \frac{1}{2} \left[\frac{B_5 - B_3}{k^4 - k^2} - \frac{B_4 - B_2}{k^3 - k} \right] \quad (36)$$

$$f_0^{(0)} = B_1 - (f_1^{(0)} + f_2^{(0)} + f_3^{(0)} + f_4^{(0)}) \quad (37)$$

1.5 数值稳定性

方程(27)可写成

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} u^2 + u \right) = \mu \frac{\partial^3}{\partial x^2 \partial t} u + O(\epsilon^3) \tag{38}$$

而截断误差为

$$R = O(\epsilon^3) = -\frac{1}{2} \frac{\partial^4}{\partial x^4} \left(\frac{1}{3} u^3 \right) - \frac{1}{2} \frac{\partial^4}{\partial x^4} u^2 - \frac{1}{3} \frac{\partial^4}{\partial x^4} u + O(\epsilon^4) \tag{39}$$

稳定条件^[3]:粘性主项系数满足 $\mu_1 > 0, \mu_2 > 0, \mu_3 > 0$,色散条件 $\mu > 0$ 自然满足。图 2 给出了 $\mu > 0$ 的取值范围。

2 数值模拟

考虑正则长波方程的初边值问题^[10]

$$\begin{aligned} \frac{\partial}{\partial t} (u - \mu \frac{\partial^2 u}{\partial x^2}) + \frac{\partial G(u)}{\partial x} &= 0 \\ u(a, t) = u(b, t) &= 0 \\ u(x, 0) &= u_0(x) \\ a < x < b, \quad 0 < t < T \end{aligned} \tag{41}$$

其中 $G(u) = u + u^2/2, \mu = 1.0$,考察孤立波的传播,选择 $u_0(x) = 3(c_0 - 1) (\text{sech } X_0)^2$,其中 $X_0 = \sqrt{(c_0 - 1)/(4c_0)}(x - d_0), c_0 = 2, d_0 = 8$.

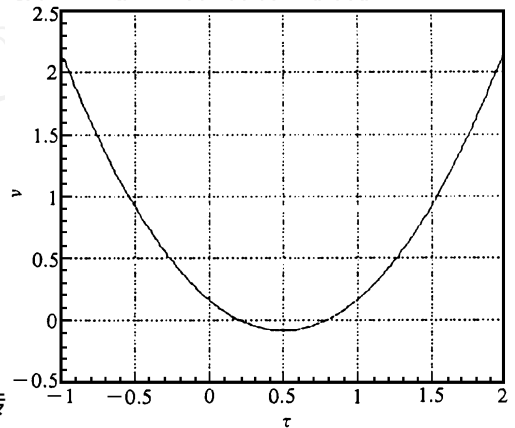


图 2 ν 与 τ 的关系曲线

Fig. 2 The curve of ν versus τ

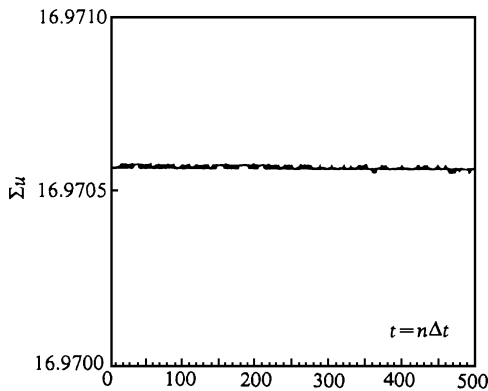


图 3 总粒子数随时间的变化

Fig. 3 Total number of particles versus t

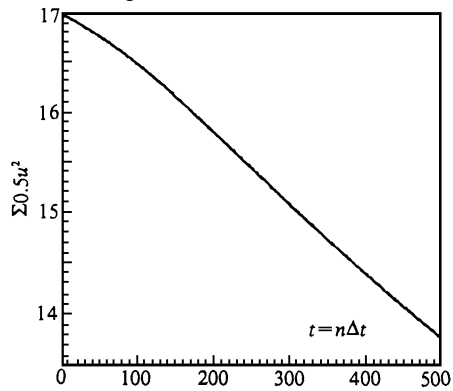


图 4 总能量随时间的变化,其中 $c = 50.0,$

$\mu = 1.0$, 结点数为 $m = 200$.

Fig. 4 Total energy of particles versus t , where

$c = 50.0, \mu = 1.0$, lattice size = 200

计算结果表明,单孤立波在传播过程中物理量(总粒子数) $\sum_{j=0}^m u(x_j, t)$ 是守恒的(图 3),而总能量($\sum_{j=1}^m \frac{1}{2} u^2(x_j, t)$) (图 4) 稍有耗散^[11]。在传播过程中波的形状保持不变(图 5),这是符合经典结果的。

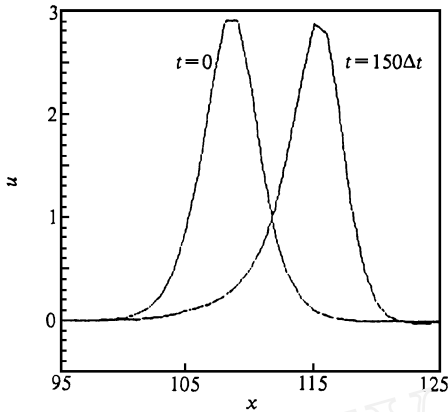


图 5 单孤立波的传播过程,其中 $c = 50.0$,
 $\mu = 1.0$, $m = 200$.

Fig. 5 The process of the solitary wave propagation, where $c = 50.0$, $\mu = 1.0$, lattice size = 200

3 结论

1991年, Frisch U 指出适当增加高阶矩的要求可以用来构造复杂问题的格子气模型^[12]。我们在此基础上,应用分布函数的 Chapman-Enskog 展开和多重尺度技术,保留多分布函数 $f^{(3)}$,得到了精度较高的 RLW 方程。应当指出的是,我们将此方法系统化,提出了时间尺度 t_0 上守恒律的概念,应用到格子 Boltzmann 方法上并且实现了模型的构造。我们的模型一方面提供了模拟 RLW 方程的算法,另一方面给出了孤立子的微观的解释。这仅是一个初步的工作,对于复杂的系统,如气体动力学的 Euler 方程,乃至 Navier-Stokes 方程的模拟将有待于解决。

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SIMULATION OF THE RLW EQUATION USING A LATTICE BOLTZMANN MODEL

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ABSTRACT A 5-bit lattice Boltzmann model is proposed for RLW equation. Using Chapman-Enskog expansion and multiscale technique, it obtains the higher order moments of equilibrium distribution function, the 3rd dispersion coefficients and 4th order viscosity. The parameters in this scheme can be determined by analysis of the stability.

KEY WORDS lattice Boltzmann method; RLW equations; multiscale method; 5-bit lattice; conservation law on time scale t_0 .