LBM单组分等温两相流-1

流体力学的基本方程

连续性方程 $\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0$ or $\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_k)}{\partial x_k}=0$

应力张量

动量方程 $\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{uu})=\rho\mathbf{F}+\nabla\cdot\boldsymbol{\sigma}$ or $\frac{\partial}{\partial t}(\rho u_j)+\frac{\partial}{\partial x_i}(\rho u_i u_j)=\rho f_j+\frac{\partial \sigma_{ij}}{\partial x_i}$

牛顿流体，应力张量的形式为 $\sigma=[-p+\lambda\nabla\cdot\mathbf{u}]\mathbf{I}+\mu\left[\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right]$ or $\sigma_{ij}=-p\delta_{ij}+\lambda\delta_{ij}\frac{\partial u_k}{\partial x_k}+\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$

$\lambda=K-\frac{2}{3}\mu$ 为第二粘性系数　K 为体积粘度

带入动量方程 $\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{uu})=-\nabla p+\rho\mathbf{F}+\nabla\cdot\left(\lambda(\nabla\cdot\mathbf{u})\mathbf{I}+\mu\left[\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right]\right)$ or

$$\frac{\partial}{\partial t}(\rho u_j)+\frac{\partial}{\partial x_i}(\rho u_i u_j)=-\frac{\partial p}{\partial x_j}+\rho f_j+\frac{\partial}{\partial x_j}\left(\lambda\frac{\partial u_k}{\partial x_k}\right)+\frac{\partial}{\partial x_i}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right]$$

$$\bar{p}=p-\left(\lambda+\frac{2}{3}\mu\right)\nabla\cdot\vec{u}$$

体积粘度的物理意义：流体发生膨胀或压缩时，平均法向应力不等于平衡态压强，二者差值正比于K

体积膨胀引起粘性应力与体积变化时的能量耗散机制有关，除高温、高频声波等极端情况外，可假设体积粘度为0（Stokes假设）

格子玻尔兹曼方法

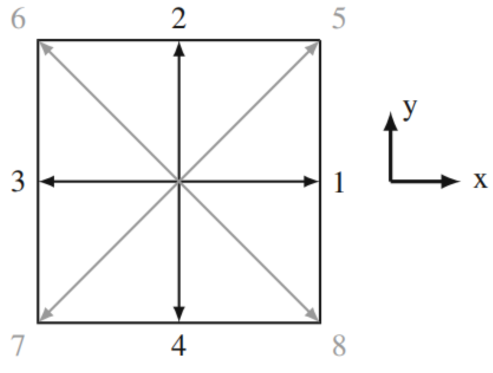
格子玻尔兹曼BGK方程（LBGK方程）：

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

碰撞步： $f_i^{\star}(\mathbf{x},t) = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$

迁移步： $f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{\star}(\mathbf{x},t)$

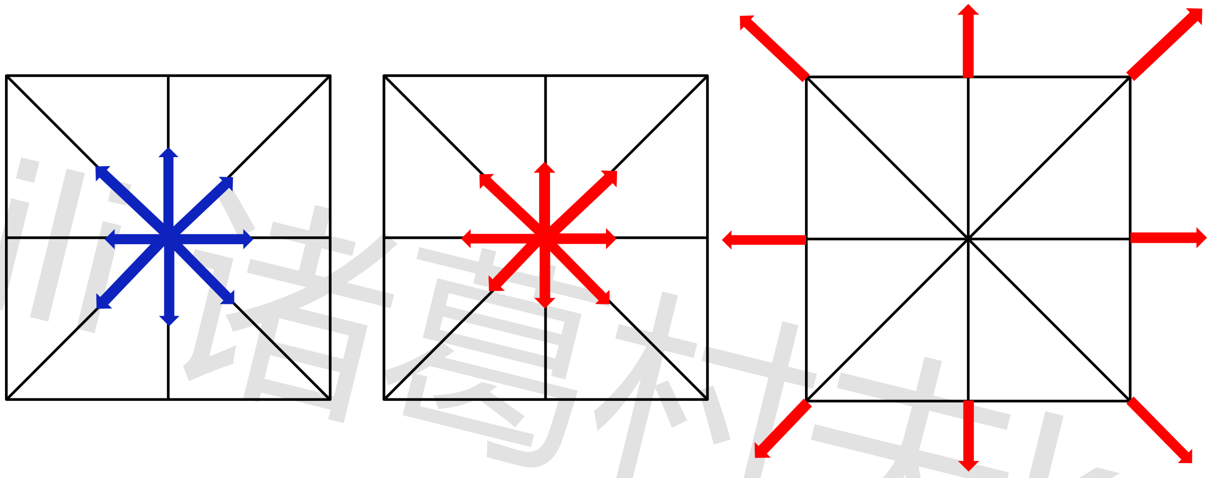
速度离散：

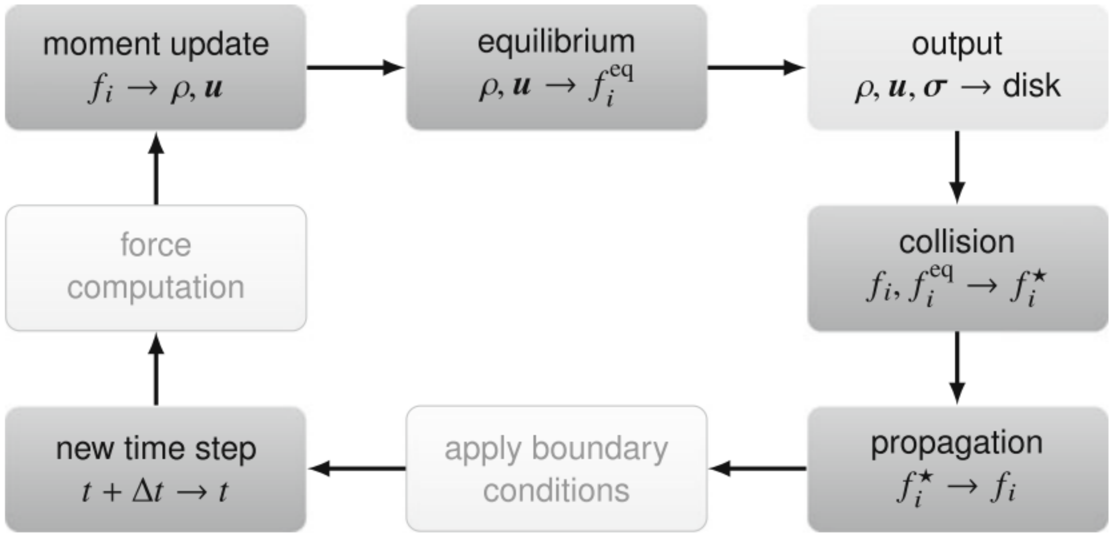


D2Q9

宏观量计算： $\sum_{i=0}^{q-1} f_i(\mathbf{x},t) = \rho(\mathbf{x},t), \quad \sum_{i=0}^{q-1} \mathbf{c}_i f_i(\mathbf{x},t) = \rho\mathbf{u}(\mathbf{x},t)$

不直接模拟宏观量的演化
而是模拟分布函数的演化，再计算宏观量





LB程序代码实施流程

格子玻尔兹曼方法

动量方程 $\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{uu})=-\nabla p+\rho\mathbf{F}+\nabla\cdot\left(\lambda(\nabla\cdot\mathbf{u})\mathbf{I}+\mu\left[\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right]\right)$

从格子玻尔兹曼方程到宏观方程：Chapman-Enskog展开

格子玻尔兹曼方程：

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t,t+\Delta t)=f_i(\mathbf{x},t)-\frac{\Delta t}{\tau}\left(f_i(\mathbf{x},t)-f_i^{\mathrm{eq}}(\mathbf{x},t)\right)+F_i$$

碰撞步： $f_i^{\star}(\mathbf{x},t)=f_i(\mathbf{x},t)-\frac{\Delta t}{\tau}\left(f_i(\mathbf{x},t)-f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$

迁移步： $f_i(\mathbf{x}+\mathbf{c}_i\Delta t,t+\Delta t)=f_i^{\star}(\mathbf{x},t)$

CE展开 →

$$\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{uu})$$

$$\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{uu})=-\nabla p+\rho\mathbf{F}+\nabla\cdot\left(\mu\left[\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right]\right)$$

$$p_{\mathrm{LBE}}=\rho c_s^2,\quad \mu=\rho c_s^2\left(\tau-\frac{\Delta t}{2}\right)\qquad c_s^2=\frac{1}{3}\left(\frac{\delta_x}{\delta_t}\right)^2$$

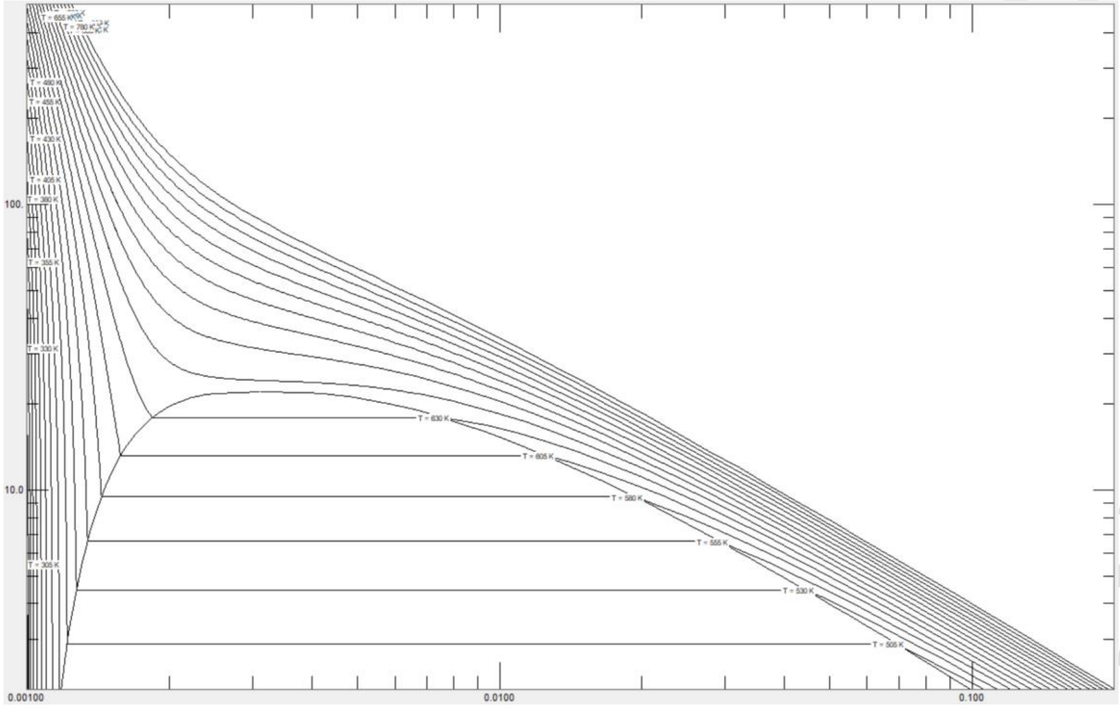
LBM求解的方程与实际待求解的方程的区别：

1. 与λ有关的项缺失（对不可压流动没有影响，但对可压缩流动有影响）
2. 宏观方程的压力项代表理想气体状态方程

格子玻尔兹曼方法单组分两相流

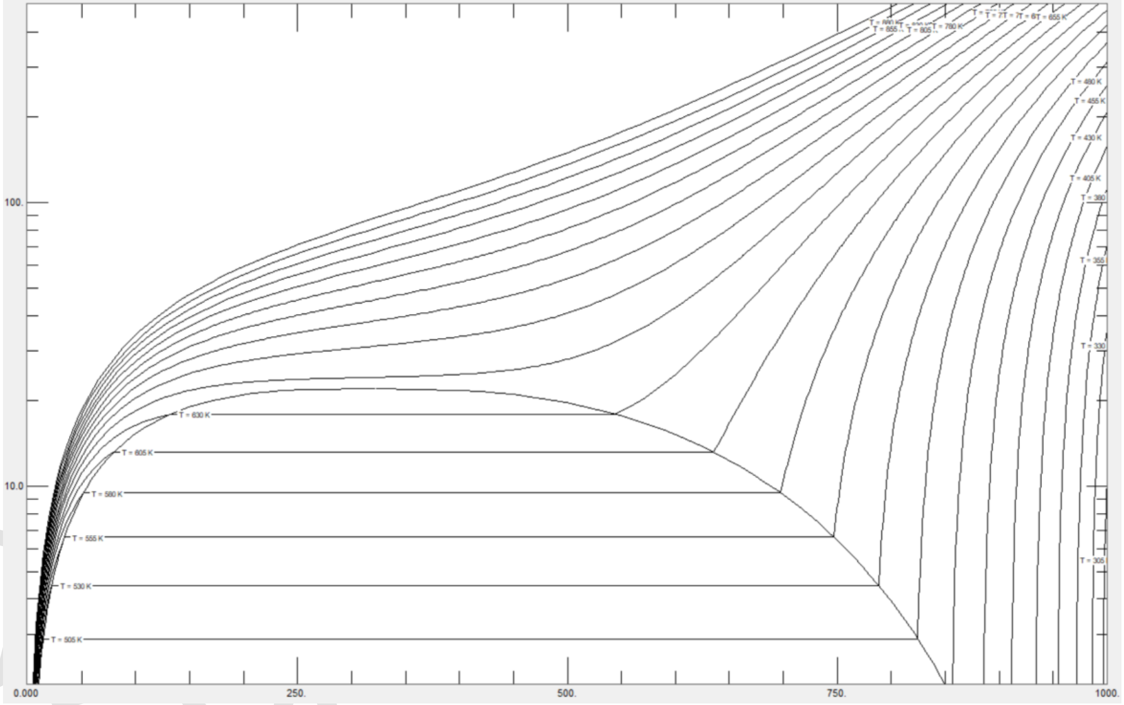
基础知识：气液相平衡（以水的p-v图为例）

P(MPa)



V(m^3/kg)

P(MPa)



ρ(kg/m^3)

$$c_s^2 = \left(\frac{\partial p}{\partial \rho} \right)_T$$

格子玻尔兹曼方法单组分两相流

```
for (int n = 0; n <= NSTEPS; n++) {
    //计算密度与压力
    compute_rho();
    compute_pressure();

    //更新伪势作用力
    compute_interaction_force();

    //计算速度
    compute_velocity();

    //碰撞
    compute_LatticeForce();
    collide();

    //迁移
    stream();
```

传统模型：

- VOF，level set等，需要追踪相界面，两相分别求解两套NS方程
- 对于气相区域，基本都采用理想气体状态方程

伪势LBM模型（pseudopotential LB model）

- 没有明确的相界面，只有密度场，全场求解同一个方程
- 无需追踪相界面，引入粒子间相互作用力实现气液相分离

伪势

$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2\sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$

伪势模型中，伪势与压力的关系为：$p_{\mathrm{EOS}} = c_s^2\rho + \dfrac{c_s^2}{2}g[\psi(\rho)]^2$

任意实际气体状态方程的引入：$p_{\mathrm{EOS}} = \dfrac{\rho RT}{1-b\rho} - a\rho^2 \Rightarrow \psi = \sqrt{\dfrac{2}{gc_s^2}\left(\dfrac{\rho RT}{1-b\rho} - a\rho^2 - \rho c_s^2\right)}$

CS EOS：$p_{\mathrm{EOS}} = \rho RT\dfrac{1+b\rho/4+(b\rho/4)^2-(b\rho/4)^3}{(1-b\rho/4)^3} - a\rho^2$

PR EOS：$p_{\mathrm{EOS}} = \dfrac{\rho RT}{1-b\rho} - \dfrac{a\alpha(T)\rho^2}{1+2b\rho-b^2\rho^2}$

密度越大，粒子间相互作用力越大，高密度区域聚集在一起（液相），低密度区域（气相）

P. Yuan, L. Schaefer, Equations of state in a lattice Boltzmann model, Phys Fluids 18 (2006) 042101.

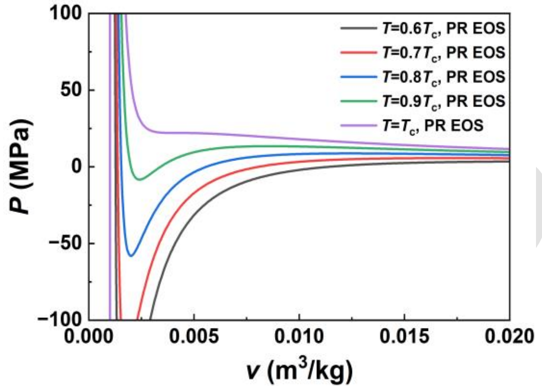
格子玻尔兹曼方法单组分两相流

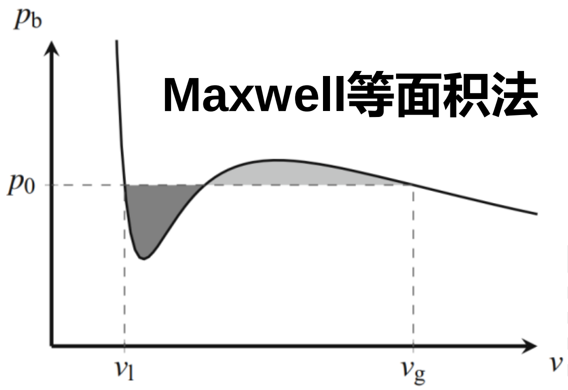
单组分两相模拟最核心的关注点：热力学一致性

热力学一致性：气液两相的吉布斯自由能相等 $G = PV - \int PdV + \varphi(T) \Rightarrow \int_{v_l}^{v_v} (p(v) - p_0)dv = 0$

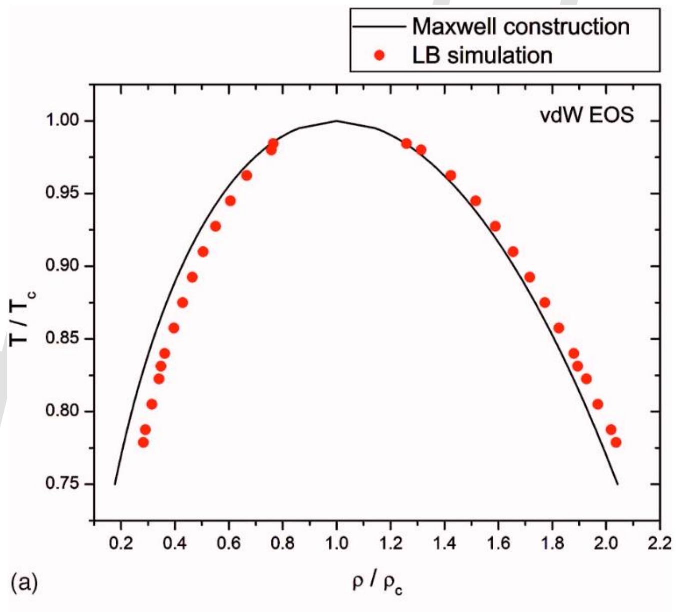
PR EOS： $p_{\mathrm{EOS}} = \dfrac{\rho RT}{1 - b\rho} - \dfrac{a\alpha(T)\rho^2}{1 + 2b\rho - b^2\rho^2}$

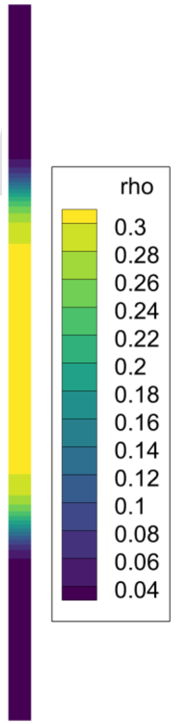
$$\mathbf{F}(\mathbf{x}) = -g\psi(\mathbf{x})c_s^2 \sum_{\alpha=1}^{N} w(|\mathbf{e}_\alpha|^2)\psi(\mathbf{x}+\mathbf{e}_\alpha)\mathbf{e}_\alpha$$






```
% PR状态方程参数
a = 1/49;
b = 2/21;
R = 1;
omega = 0.344;
Tc = (0.0778/0.45724) * (a/b);
Pc = 0.0778*Tc/b;
syms v rho Temp
alpha(Temp) = (1 + (0.37464+1.54226*omega-0.26992*omega^2)*(1-sqrt(Temp./Tc))).^2;
pressure(rho,Temp) = (rho*R*Temp)/(1-b*rho) - a*rho^2*alpha(Temp)/(1+2*b*rho-b*b*rho*rho);
d_pressure(rho,Temp) = diff(pressure, rho);
dd_pressure(rho,Temp) = diff(d_pressure, rho);
rhoc = double(vpasolve(dd_pressure(rho,Tc)==0, rho, [0, 5]));
```





遗憾的是，采用这种作用力形式并不能满足热力学一致性

P. Yuan, L. Schaefer, Equations of state in a lattice Boltzmann model, Phys Fluids 18 (2006) 042101.

格子玻尔兹曼方法单组分两相流

问题总结：

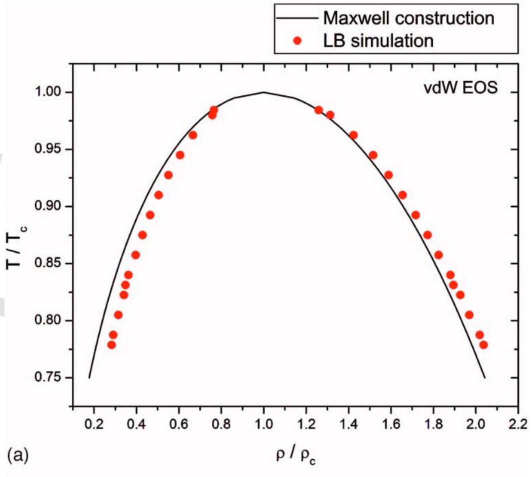
1.由LBGK方程恢复得到的宏观方程中，与λ有关的项缺失

2.由LBGK方程恢复得到的宏观方程中，压力项代表理想气体状态方程

3.采用原始的粒子间作用力形式不能满足热力学一致性

4.格子体系下的声速与实际体系下的声速不对应

5.模拟能够达到的最低温度不够低（气液密度比不够大），难以应用于实际问题



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碰撞步： $$f_i^{\star}(\mathbf{x},t) = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

迁移步： $$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{\star}(\mathbf{x},t)$$

CE展开

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u})$$

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \rho\mathbf{F} + \nabla\cdot\left(\mu\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right]\right)$$

$$p_{\mathrm{LBE}} = \rho c_s^2, \quad \mu = \rho c_s^2\left(\tau - \frac{\Delta t}{2}\right) \qquad c_s^2 = \frac{1}{3}\left(\frac{\delta_x}{\delta_t}\right)^2$$