

DPD 方法及其它无网格方法的边界条件 组会

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 - 粒子层法
 - 粒子层与反弹运动方法结合
- 2 Boundary condition in dissipative particle dynamics
 - 模型
 - 结果
- 3 A new wall boundary condition in particle methods
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- 4 An implementation of no-slip boundary conditions in DPD
 - 模型
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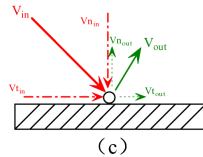
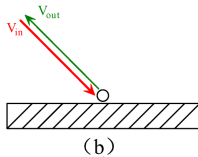
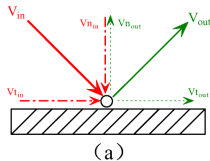
边界类型

对于所有的计算流体力学问题，边界条件都是重要的研究内容。
在无网格方法中，一般有以下几类边界条件：

- 周期边界
- 粒子层法
- 粒子反弹运动方法
 - ① 镜子映像 (Specular reflection)
 - ② 反弹映像 (bounce-back reflection)
 - ③ 麦克斯韦映像 (Maxwellian reflection)
- 粒子层与反弹运动方法结合

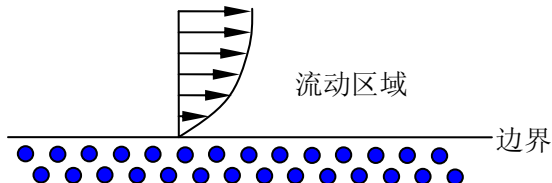
粒子反弹运动方法

粒子反弹运动方法:(a) 镜子映像 (Specular reflection); (b) 反弹映像 (bounce-back reflection); (c) 麦克斯韦映像 (Maxwellian reflection)



粒子层与反弹运动方法结合

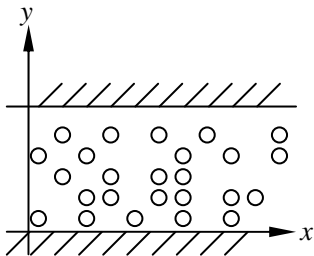
粒子层与反弹运动方法结合



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这篇文章对上图的模型分别对反弹映像的三种边界条件作了研究.

Dimensionless friction coefficient:

$$\tau = \gamma \lambda / d v_T$$

γ : friction coefficient. λ : average distance between particles. d : spatial dimension(=2). $v_T = \sqrt{k_b T / m}$

The two components of temperature:

$$T^x = \sum_i m_i v_{x_i}^2, T^y = \sum_i m_i v_{y_i}^2$$

结果

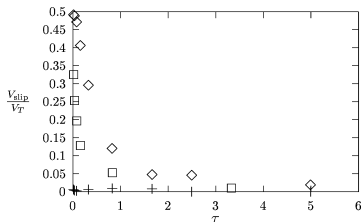


Fig. 1. Slip velocity at the wall for the specular (diamonds), Maxwellian (squares), and bounce back (crosses) reflections versus τ .

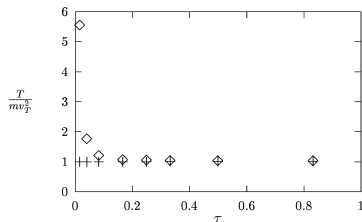
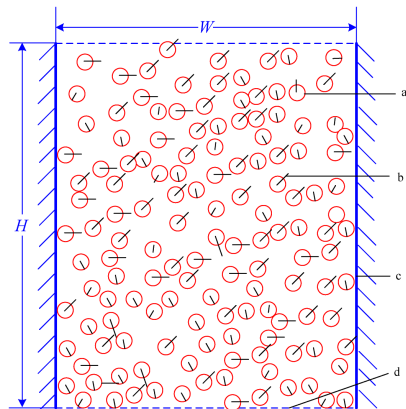
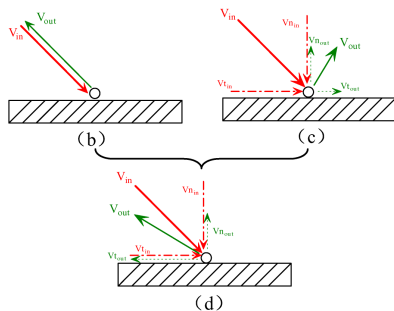


Fig. 2. T^x (diamonds) and T^y (crosses) versus τ when $T = 1$.

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与边界作用前后速度分别为

$$\mathbf{V} = v_n \mathbf{n} + v_t \boldsymbol{\tau}, \mathbf{V}' = -[(1 - \alpha)v_n + \alpha u] \mathbf{n} - v_t \boldsymbol{\tau}$$

其中 u 服从

$$F(u) = 2\beta^2 u \exp(-\beta^2 u^2), \beta = (2k_b/mT_w)^{-1/2}$$

Pseudo-particle modeling (PPM): 粒子与粒子作用前后速度 v_1, v_{10}

$$v_1 = v_{10} - \frac{2m_2}{m_1 + m_2} \cdot \frac{(v_{10} - v_{20}) \cdot (P_1 - P_2)}{|P_1 - P_2|^2} (P_1 - P_2)$$

两边界的温度相等的结果

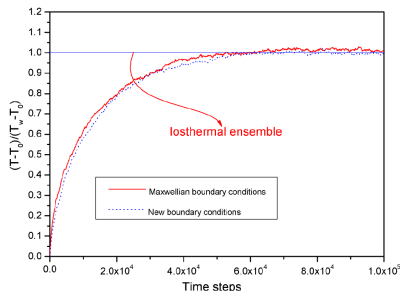


Fig. 3. The temporal evolution of temperature in the bulk fluid between walls of constant temperature.

两边界的温度相等

$$T_1 = \frac{mv_1^2}{2k_b} = T_2 = \frac{mv_2^2}{2k_b} > T_0$$

两边界的温度不等的结果

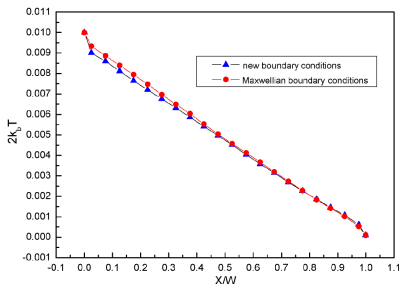
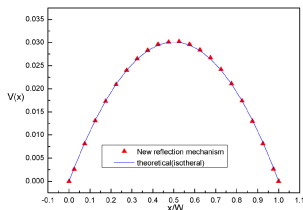


Fig. 4. Temperature distributions for heat conduction in a channel.

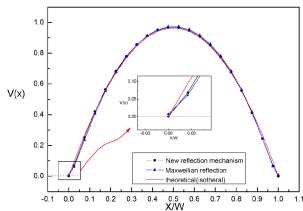
两边界的温度不等

$$T_1 = \frac{mv_1^2}{2k_b} > T_0 > T_2 = \frac{mv_2^2}{2k_b}$$

加重力场的结果

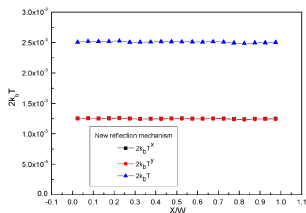


(a)

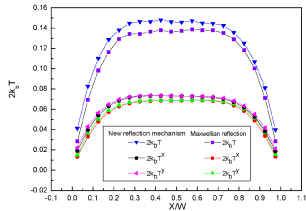


(b)

Fig. 5. Results from the simulation of plane Poiseuille flow. (a) Driven by $g = 2e-7$. (b) Driven by $g = 5e-5$.



(a)



(b)

Fig. 6. Temperature distributions in a plane Poiseuille flow. (a) Driven by $g = 2e-7$. (b) Driven by $g = 5e-5$.

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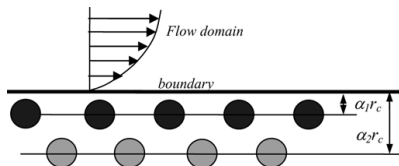


Fig. 1 The structure of the double layer

α_1, α_2 满足:

$$0 < \alpha_1 < \alpha_2$$

穿过边界的粒子

$$v_{new} = 2v_{wall} - v_{old}$$

$$r_{new} = r_{old} + 2d_r \mathbf{n}_w$$

边界单粒子层

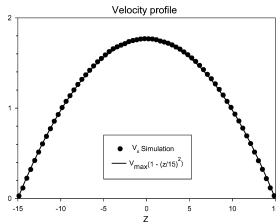


Fig. 2 The fully developed velocity and the Navier-Stokes solution

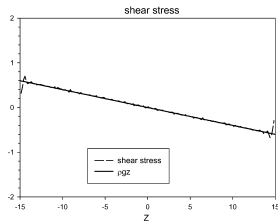


Fig. 4 The shear stress and the analytical solution

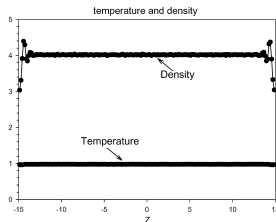


Fig. 3 The temperature and density

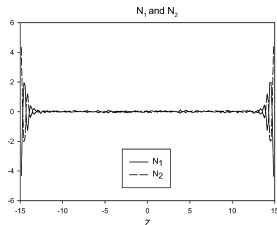


Fig. 5 The first and second normal stress difference

边界双粒子层

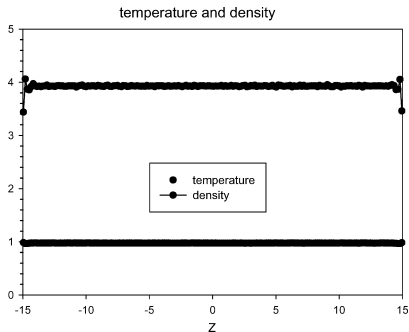


Fig. 6 The temperature and density in case of using a double layer wall

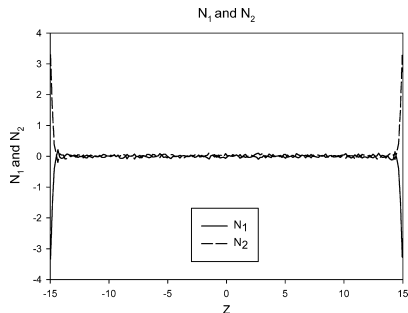


Fig. 7 The first and second normal stress difference

Thank You!!!