Boundary Conditions
in lattice Boltzmann method

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Outline

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Definitions

- Boundary Value Problem $\begin{cases} \text{Partial Differential Equation} \\ \text{Boundary Condition} \end{cases}$

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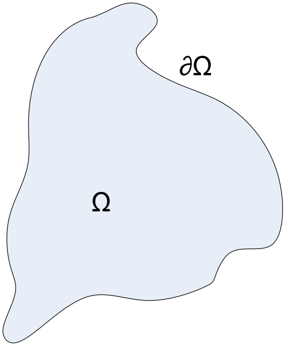
e.g. Poisson equation:

$$\left\{ \begin{array}{ll} \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = f(x, y), & \text{in } \Omega \\ \varphi = \varphi_b, & \text{on } \partial\Omega \end{array} \right.$$



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→ Robin Boundary Condition

$$g\varphi + h\frac{\partial\varphi}{\partial n} = \varphi_b \quad \text{on } \partial\Omega$$

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- Steady isothermal and incompressible Navier-Stokes equations

$$\left\{ \begin{array}{c} (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu\triangle\mathbf{u} + \mathbf{a} \\ \nabla\cdot\mathbf{u} = 0 \end{array} \right. \quad \text{in } \Omega$$

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$$\mathbf{u} = \mathbf{u}_b \quad \text{on } \partial\Omega$$

- Boundary Condition on fluid boundaries

$$\mathbf{u} = \mathbf{u}_{in} \quad \text{on } \partial\Omega$$

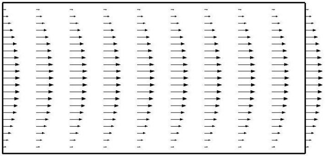
or

$$\left\{ \begin{array}{c} -p + \nu\frac{\partial u_n}{\partial n} = (F_n)_{in} \\ \nu\frac{\partial u_t}{\partial n} = (F_t)_{in} \end{array} \right. \quad \text{on } \partial\Omega$$

Definitions

- Periodic or Cyclic Boundary Conditions

$$\mathbf{u}(x,y) = \mathbf{u}(x+L,y) \quad \text{in } \Omega \quad \Rightarrow \quad \mathbf{u}_{in} = \mathbf{u}_{out} \quad \text{on } \partial\Omega$$



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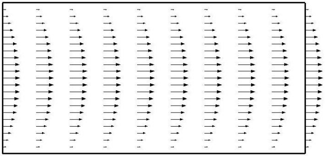
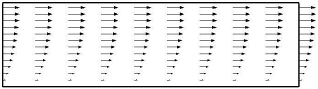


- Symmetry Boundary Conditions

$$\mathbf{u}\cdot\mathbf{n} = 0 \quad \text{and} \quad \frac{\partial \mathbf{u}}{\partial n} = 0 \quad \text{on } \partial\Omega$$



Outline

Introduction and motivation

- Lattice Boltzmann method (LBM)

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = f_\alpha(\mathbf{x}, t) - \omega(f_\alpha - f_\alpha^{(eq)})|_{(\mathbf{x},t)} \quad \text{in } \Omega$$

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  → f_α set in a higher DoF system than $\{\rho, \mathbf{u}, \mathbf{\Pi}\}$, hence:

    - Trivial: $f_\alpha \longrightarrow \{\rho, \mathbf{u}, \mathbf{\Pi}\}$
    - Complex: $\{\rho, \mathbf{u}, \mathbf{\Pi}\} \longrightarrow f_\alpha$

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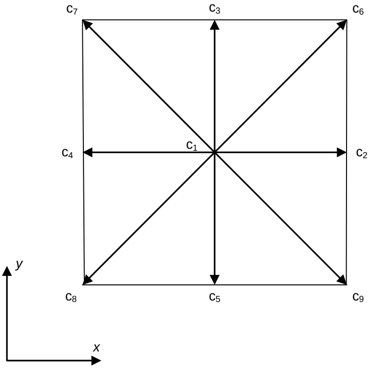
  → Incorrect upscaling $\longrightarrow$ Unwanted behavior, e.g. Knudsen layers

Lattice structure



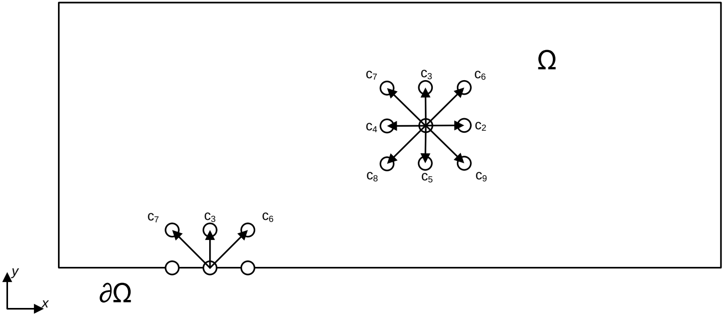
- D2Q9 model

$$
\begin{aligned}
\mathbf{c}_1 &= (0, 0) \\
\mathbf{c}_2 &= (1, 0) \\
\mathbf{c}_3 &= (0, 1) \\
\mathbf{c}_4 &= (-1, 0) \\
\mathbf{c}_5 &= (0, -1) \\
\mathbf{c}_6 &= (1, 1) \\
\mathbf{c}_7 &= (-1, 1) \\
\mathbf{c}_8 &= (-1, -1) \\
\mathbf{c}_9 &= (-1, -1)
\end{aligned}
$$

Definitions

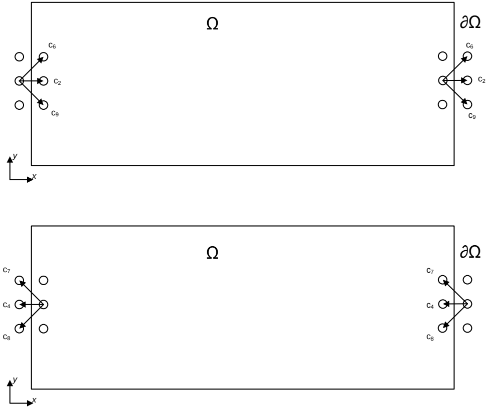
→ $\mathbf{x}$ is a fluid node if $\forall \mathbf{c}$ so that $\mathbf{x} + \mathbf{c}\Delta t \in \{\Omega \bigcup \partial\Omega\}$

→ $\mathbf{x}$ is a boundary node if $\exists \mathbf{c}$ so that $\mathbf{x} + \mathbf{c}\Delta t \notin \{\Omega \bigcup \partial\Omega\}$



Periodic Boundary Conditions

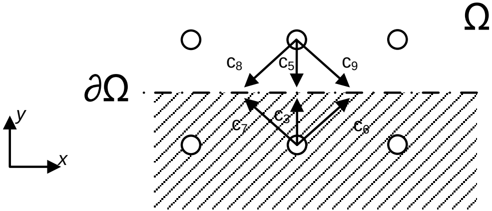
$$\text{Periodicity} \rightarrow \quad \mathbf{u}_{in} = \mathbf{u}_{out} \quad \text{on } \partial\Omega$$



Symmetry Boundary Conditions

Symmetry $\rightarrow$ $\quad \mathbf{u} \cdot \mathbf{n} = 0 \quad \text{and} \quad \frac{\partial \mathbf{u}}{\partial n} = 0 \quad \text{on } \partial\Omega$

(also called free-slip boundary)



Bounceback Boundary Conditions

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A hard wall reflects particles back to where they originally came from

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A hard wall reflects particles back to where they originally came from

As a result:

$\rightarrow$ There is no flux crossing the wall, *i.e.* the wall is impermeable

$\rightarrow$ There is no relative transverse motion between fluid and wall, *i.e.* no-slip at the wall

Bounceback Boundary Conditions

REMEMBER: LBM algorithm can be operated in 2 steps:

→ Collision step:

$$\tilde{f}_\alpha(\mathbf{x}, t) = f_\alpha(\mathbf{x}, t) - \omega(f_\alpha - f_\alpha^{(eq)})|_{(\mathbf{x},t)}$$

→ Streaming step:

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = \widetilde{f}_\alpha(\mathbf{x}, t)$$

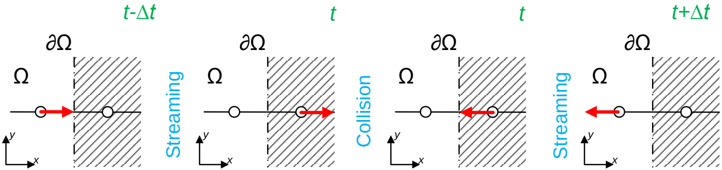
Bounceback Boundary Conditions

The Bounceback method can be implemented following 2 reasonings:

- **Full-way bounceback:**
  - $\rightarrow$ inversion of particle velocity takes place during the **collision step**
- **Half-way bounceback:**
  - $\rightarrow$ inversion of particle velocity takes place during the **streaming step**

Bounceback Boundary Conditions

Full-way Bounceback: $\tilde{f}_{\bar{\alpha}}(\mathbf{x}_b, t) = f_\alpha(\mathbf{x}_b, t)$



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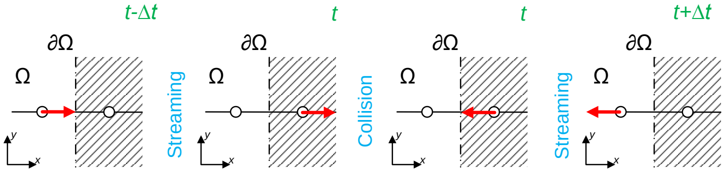
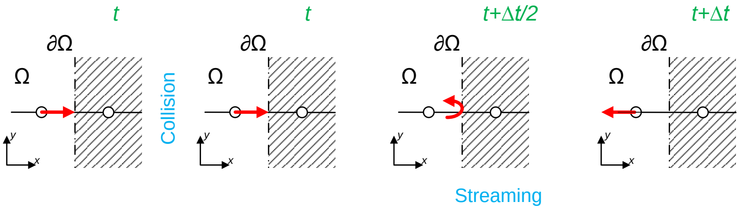
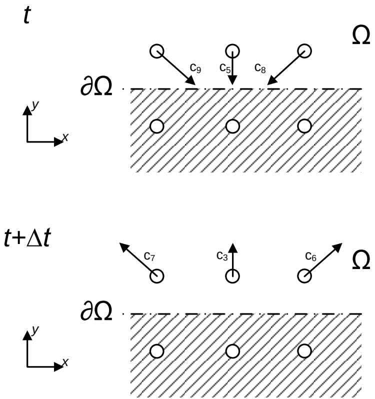


Half-way Bounceback: $f_{\bar{\alpha}}(\mathbf{x}_f, t + \Delta t) = \tilde{f}_\alpha(\mathbf{x}_f, t)$



Bounceback Boundary Conditions

Half-way bounceback in 2D:



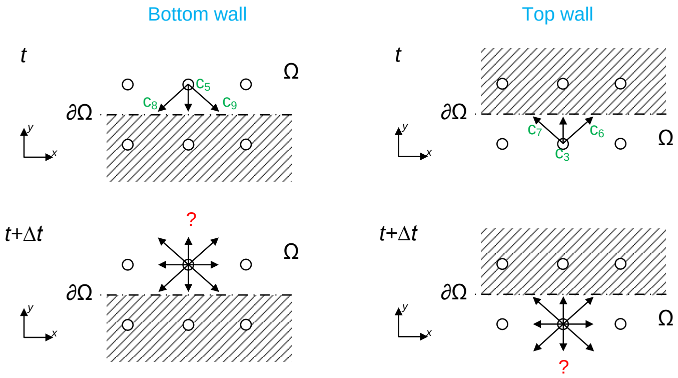
Bounceback Boundary Conditions: summary

- **Pros**
  - → Mass is exactly conserved
  - → Stable for ω close to 2 (i.e. for high Re)
  - → Local
  - → Flexibility in handling wall, edges, corners both in 2D and 3D
  - → Very simple to implement from a programming viewpoint
- **Cons**
  - → Velocity accuracy may decrease from 2^{nd} to 1^{st}
  - → Pressure accuracy may decrease from 1^{st} to 0^{th}
  - → In SRT model momentum is not exactly conserved (viscosity dependent slip velocity), which is equivalent to say the boundary location is not exactly defined (viscosity dependent slip length)

Bounceback Boundary Conditions: Exercise

Question:

Use the half-way bounceback scheme to find the unknown populations at $t + \Delta t$



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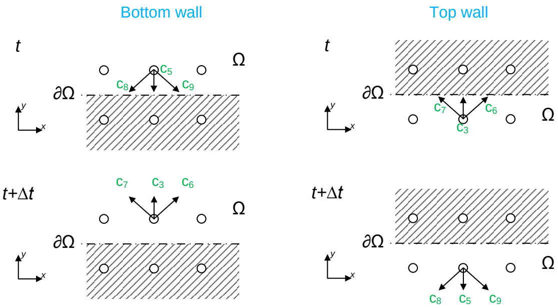

Momentum exchange

- Force (per unit volume):

$$\mathbf{F}\big|_{(t+\frac{\Delta t}{2})} = \frac{\Delta \mathbf{p}}{\Delta t}\Big|_{(t+\frac{\Delta t}{2})} = \frac{1}{\Delta t}(\mathbf{p}(t+\Delta t) - \mathbf{p}(t))$$

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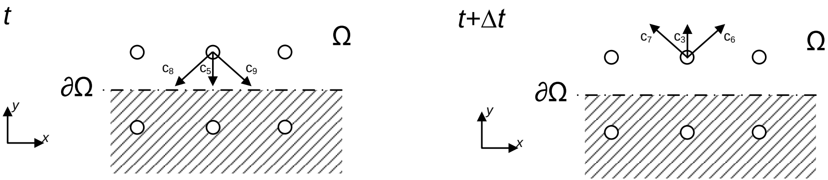

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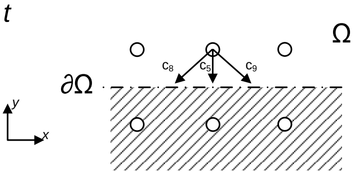

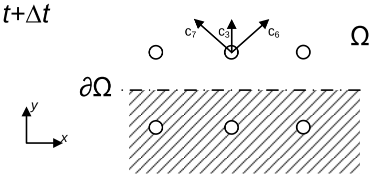

- Momentum exchange (per unit volume) between the fluid/wall surface:

$$\Delta \mathbf{p}(\mathbf{x}, t+\frac{\Delta t}{2}) = \sum_{\alpha} \left[(\mathbf{c}_{\bar{\alpha}}) f_{\bar{\alpha}}(\mathbf{x}, t+\Delta t) - (\mathbf{c}_{\alpha}) \tilde{f}_{\alpha}(\mathbf{x}, t) \right]$$

Momentum exchange

- Momentum exchange between the fluid/wall surface:

$$\Delta \mathbf{p}(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -\sum_{\alpha} \mathbf{c}_\alpha \left[f_{\bar{\alpha}}(\mathbf{x}, t + \Delta t) + \tilde{f}_\alpha(\mathbf{x}, t) \right]$$

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Remember: Half-way Bounceback: $f_{\bar{\alpha}}(\mathbf{x}_f, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_f, t)$

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$$\Rightarrow \ \Delta \mathbf{p}(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -2 \sum_{\alpha} \mathbf{c}_{\alpha} \tilde{f}_{\alpha}(\mathbf{x}, t)$$

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$$\Rightarrow \; \Delta\mathbf{p}(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -2 \sum_{\alpha} \mathbf{c}_{\alpha} \tilde{f}_{\alpha}(\mathbf{x}, t)$$

Force on the fluid due to the wall :

$$\mathbf{F}(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -2 \frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} \sum_{\alpha} \mathbf{c}_{\alpha} \tilde{f}_{\alpha}(\mathbf{x}, t)$$

Transverse force on the fluid due to the bottom wall

$$F_x(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} \sum_{\alpha} (c_\alpha)_x \tilde{f}_\alpha(\mathbf{x}, t)$$

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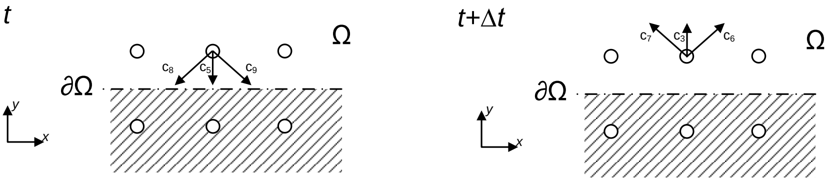

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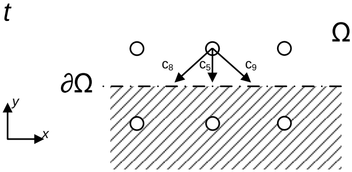

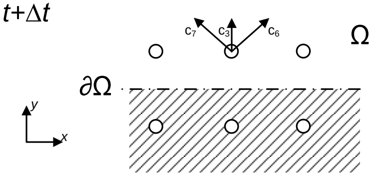

Transverse force by bottom wall:

$$F_x(\mathbf{x}, t + \frac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} (\tilde{f}_9 - \tilde{f}_8)|_{(\mathbf{x},t)}$$

Normal force on the fluid due to the bottom wall

$$F_y(\mathbf{x}, t + \frac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} \sum_{\alpha} (c_\alpha)_y \tilde{f}_\alpha(\mathbf{x}, t)$$

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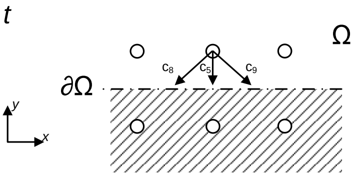
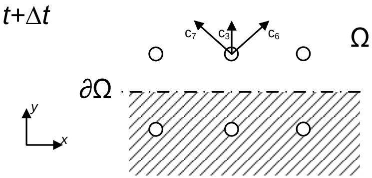
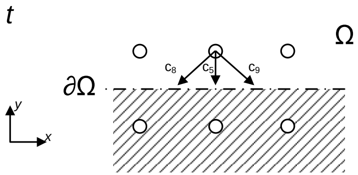
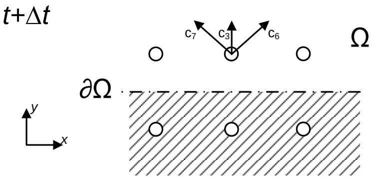




Normal force on the fluid due to the bottom wall

$$F_y(\mathbf{x}, t+\frac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t}\sum_{\mathbf{x}_b \in S}\sum_{\alpha}(c_\alpha)_y \tilde{f}_\alpha(\mathbf{x}, t)$$





Normal force by bottom wall:

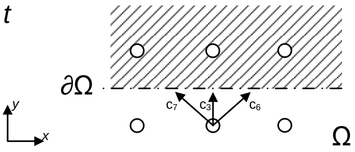
$$F_y(\mathbf{x}, t+\frac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t}\sum_{\mathbf{x}_b \in S}(\tilde{f}_5 + \tilde{f}_8 + \tilde{f}_9)|_{(\mathbf{x},t)}$$

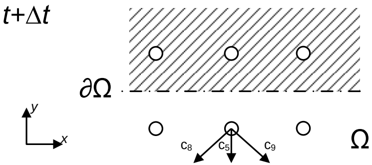
Momentum exchange: Exercise

Question:

Write the formulas of the transverse and normal forces at the top wall

Remember:





Momentum exchange: Exercise

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Solution:

- Transverse force by **top wall**:

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- Normal force by **bottom wall**:

$$F_y(\mathbf{x}, t + \tfrac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} (\tilde{f}_3 + \tilde{f}_6 + \tilde{f}_7)|_{(\mathbf{x},t)}$$

Exercise I

Exercise I:

Poiseuille flow with bounceback walls

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- The solution of the Navier-Stokes not only requires the no-slip velocity condition on walls but also demands these equations to be valid near the wall

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- The solution of the Navier-Stokes not only requires the no-slip velocity condition on walls but also demands these equations to be valid near the wall

- Taking advantage of the Chapman-Enskog expansion...

  $$f = f^{(0)}(\rho, \mathbf{u}) + \epsilon f^{(1)}(\nabla \mathbf{u}) + O(\epsilon^2)$$

- ...it can be shown:

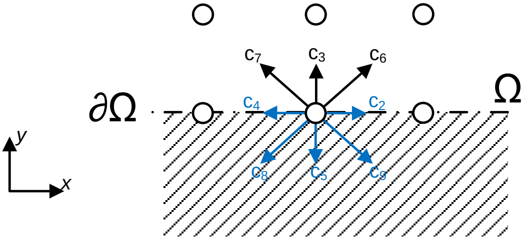
  $$f_\alpha^{(0)} = w_\alpha \left(\rho + \frac{\mathbf{c}_\alpha}{c_s^2} \cdot \mathbf{u} + \frac{(\mathbf{c}_\alpha \mathbf{c}_\alpha - c_s^2 \mathbf{I})}{2c_s^4} : \mathbf{uu} \right)$$

  $$f_\alpha^{(1)} = -w_\alpha \frac{(\mathbf{c}_\alpha \mathbf{c}_\alpha - c_s^2 \mathbf{I})}{\omega c_s^2} : \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)$$

Zou He boundary condition

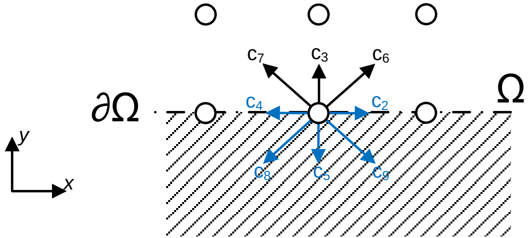
- → Boundary node and solid node coincide
- → Only unknown incoming populations are modified
- → Set ρ or $\mathbf{u}$ in $f_\alpha^{(0)}(\rho, \mathbf{u})$
- → Construct $f_\alpha^{(1)}$ from the symmetry requirement

Zou He velocity boundary condition



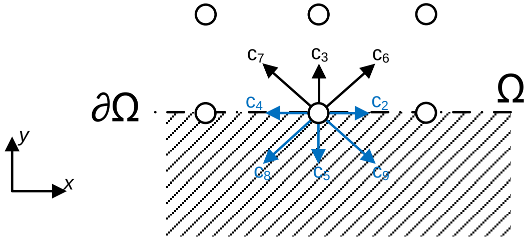
- Known:
  - $\rightarrow$ $\mathbf{u} = \mathbf{0}$
  - $\rightarrow$ $f_\alpha = (f_1, f_2, f_4, f_5, f_8, f_9)$

Zou He velocity boundary condition



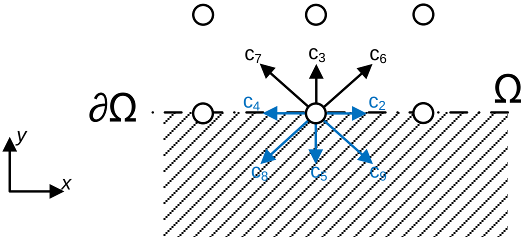
- Known:
  - $\rightarrow$ $\mathbf{u} = \mathbf{0}$
  - $\rightarrow$ $f_\alpha = (f_1, f_2, f_4, f_5, f_8, f_9)$
- Unknown (4 variables):
  - $\rightarrow$ ρ
  - $\rightarrow$ $f_\alpha = (f_3, f_6, f_7)$

Zou He velocity boundary condition



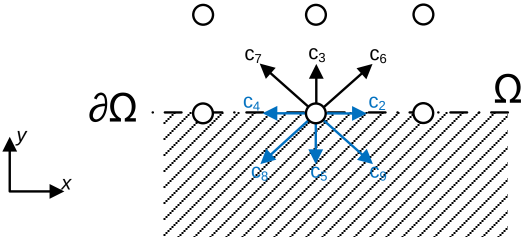
- Known:
  - $\rightarrow$ $\mathbf{u} = \mathbf{0}$
  - $\rightarrow$ $f_\alpha = (f_1, f_2, f_4, f_5, f_8, f_9)$
- Unknown (4 variables):
  - $\rightarrow$ ρ
  - $\rightarrow$ $f_\alpha = (f_3, f_6, f_7)$
- 3 Equations (2 linearly independent):
  - $\rightarrow$ $\sum f_\alpha = \rho$
  - $\rightarrow$ $\sum \mathbf{c}_\alpha f_\alpha = \mathbf{u}$

Zou He velocity boundary condition



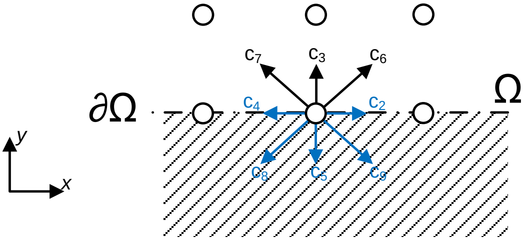
- Symmetry of $f_\alpha^{(1)}$ (3 equations):
  - $\rightarrow$ Bounceback of non-equilibrium populations

Zou He velocity boundary condition



- Symmetry of $f_\alpha^{(1)}$ (3 equations):
  - $\rightarrow$ Bounceback of non-equilibrium populations
- Introduce extra variable (problem overspecified):
  - $\rightarrow$ Transverse momentum correction N_{xy}

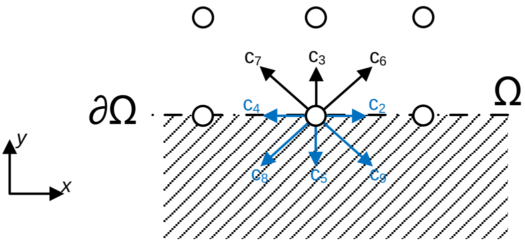
Zou He velocity boundary condition



- Symmetry of $f_\alpha^{(1)}$ (3 equations):
  - $\rightarrow$ Bounceback of non-equilibrium populations
- Introduce extra variable (problem overspecified):
  - $\rightarrow$ Transverse momentum correction N_{xy}
- Problem is well specified:
  - $\rightarrow$ 6 eqs. and 6 unknowns

Zou He velocity boundary condition

1) Computing ρ...



- Population velocity set at boundary node:

  $\rightarrow \ C_+ = \{\mathbf{c}_3, \mathbf{c}_6, \mathbf{c}_7\}$

  $\rightarrow \ C_0 = \{\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_4\}$

  $\rightarrow \ C_- = \{\mathbf{c}_5, \mathbf{c}_8, \mathbf{c}_9\}$

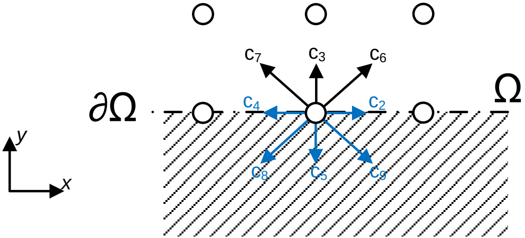
- Use the two velocity moments:

  $\rightarrow \ \sum f_\alpha = \rho$

  $\rightarrow \ \sum (c_\alpha)_y f_\alpha = u_y$

Zou He velocity boundary condition

1) Computing ρ...

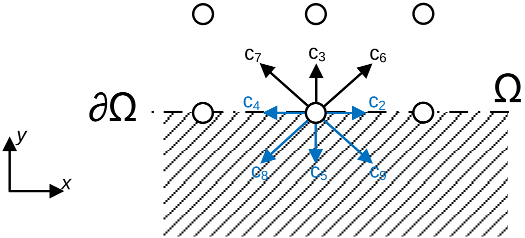


- Relate the two velocity moments:

$$\begin{cases} \rho = \rho_+ + \rho_0 + \rho_- \\ u_y = \rho_+ - \rho_- \end{cases}$$

Zou He velocity boundary condition

1) Computing ρ...



- Relate the two velocity moments:

$$\begin{cases} \rho = \rho_+ + \rho_0 + \rho_- \\ u_y = \rho_+ - \rho_- \end{cases}$$

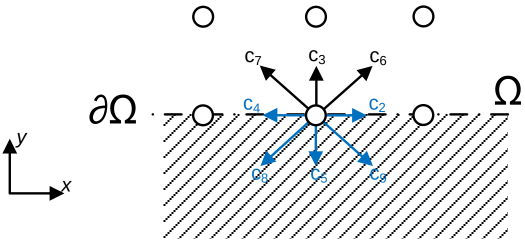
- Solution:

$$\rho = u_y + \rho_0 + 2\rho_-$$

i.e. $\rho = u_y + (f_1 + f_2 + f_4) + 2(f_5 + f_8 + f_9)$

Zou He velocity boundary condition

2) Computing $\{f_3, f_6, f_7\}$**...**



- Non-equilibrium bounceback with transverse momentum correction:

$$f_3 - f_3^{(0)} = f_5 - f_5^{(0)}$$

$$f_6 - f_6^{(0)} = f_8 - f_8^{(0)} + N_{xy}$$

$$f_7 - f_7^{(0)} = f_9 - f_9^{(0)} - N_{xy}$$

Zou He velocity boundary condition

2) Computing $\{f_3, f_6, f_7\}$**...**

Solution for the unknown incoming populations:

$$f_3 = f_5 + \frac{2}{3}u_y$$

$$f_6 = f_8 + \frac{1}{2}(f_4 - f_2) + \frac{1}{6}u_y + \frac{1}{2}u_x$$

$$f_7 = f_9 - \frac{1}{2}(f_4 - f_2) + \frac{1}{6}u_y - \frac{1}{2}u_x$$

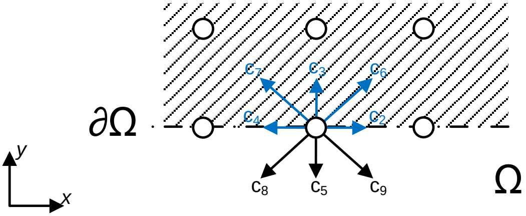
Zou He boundary condition

- **Pros**
  - → Local
  - → Velocity is 2nd order accurate
  - → Pressure accuracy is (at worst) 1st order accurate
  - → In SRT model momentum is conserved (up to 2nd order)
- **Cons**
  - → Unstable when $\omega \longrightarrow 0$
  - → Mass is not exactly conserved (2nd order accurate)
  - → Flexibility in handling wall, edges and corners or 2D and 3D domains are being modeled
  - → Not so simple to implement (compared to bounceback)

Zou He boundary condition: Exercise

Question:

Use the Zou He procedure to find ρ and the unknown populations at the top wall



Zou He boundary condition: Exercise

Question:

Use the Zou He procedure to find ρ and the unknown populations at the top wall

Solution:

$$\rho = -u_y + (f_1 + f_2 + f_4) + 2(f_3 + f_6 + f_7)$$

$$f_5 = f_3 - \frac{2}{3}u_y$$

$$f_8 = f_6 + \frac{1}{2}(f_2 - f_4) - \frac{1}{6}u_y - \frac{1}{2}u_x$$

$$f_9 = f_7 - \frac{1}{2}(f_2 - f_4) - \frac{1}{6}u_y + \frac{1}{2}u_x$$

Exercise II

Exercise II:

Poiseuille flow Zou He walls

Outline

Bounceback vs. Zou He

BC scheme	Bounceback	Zou He

Bounceback vs. Zou He

BC scheme	Bounceback	Zou He
Boundary location	Halfway	On node

Bounceback vs. Zou He

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Bounceback vs. Zou He

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Mass conservative	Yes	Only 2^{nd}

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Mass conservative	Yes	Only 2^{nd}
Viscosity independent	Not in SRT	Yes

Bounceback vs. Zou He

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Mass conservative	Yes	Only 2^{nd}
Viscosity independent	Not in SRT	Yes
Flexibility	Yes	Not as flexible

Bounceback vs. Zou He

BC scheme	Bounceback	Zou He
Boundary location	Halfway	On node
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Velocity accuracy	2^{nd} to 1^{st}	2^{nd}
Pressure accuracy	1^{st} to 0^{th}	1^{st}
Mass conservative	Yes	Only 2^{nd}
Viscosity independent	Not in SRT	Yes
Flexibility	Yes	Not as flexible
Coding simplicity	Yes	Not as simple