Boundary Conditions
in lattice Boltzmann method

Goncalo Silva
Department of Mechanical Engineering
Instituto Superior Técnico (IST)
Lisbon, Portugal

INSTITUTO SUPERIOR TÉCNICO

Outline

1. Introduction
   - Boundary Value Problems
2. Motivation
   - Navier-Stokes Boundary Conditions
3. Lattice Boltzmann Boundary Conditions
   - Problem definition
   - Boundaries in LBM
   - Particulate dynamics
   - Using Chapman-Enskog
4. Summary

Outline

Definitions

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

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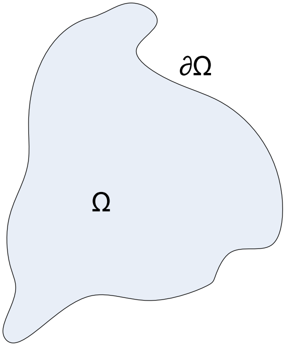
e.g. Poisson equation:

$$\begin{cases} \dfrac{\partial^2 \varphi}{\partial x^2} + \dfrac{\partial^2 \varphi}{\partial y^2} = f(x, y), & \text{in } \Omega \\ \varphi = \varphi_b, & \text{on } \partial\Omega \end{cases}$$



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$\rightarrow$ Robin Boundary Condition

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

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Definitions

- 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

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

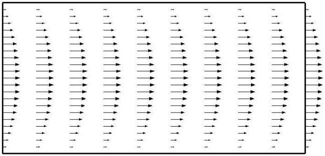
or

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

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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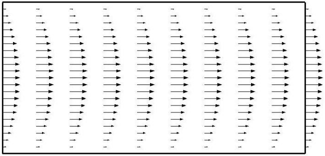
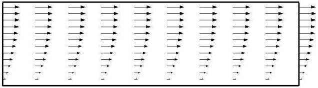


- Symmetry Boundary Conditions

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



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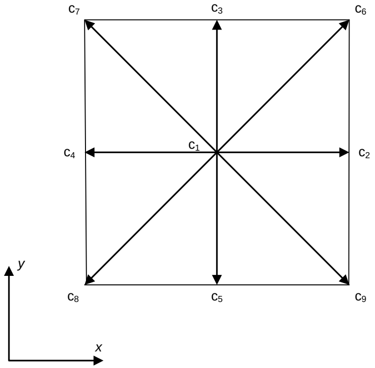
  → Incorrect upscaling $\longrightarrow$ Unwanted behavior, e.g. Knudsen layers

Lattice structure



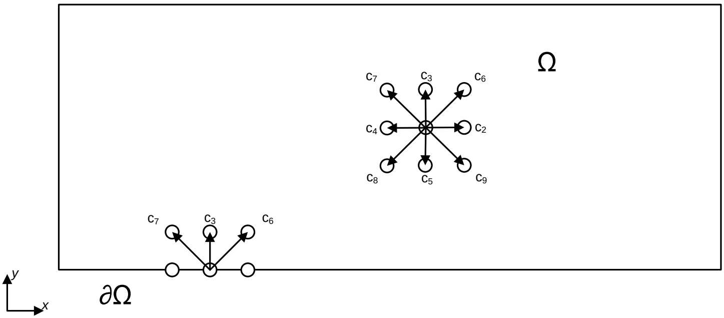
- D2Q9 model

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

Definitions

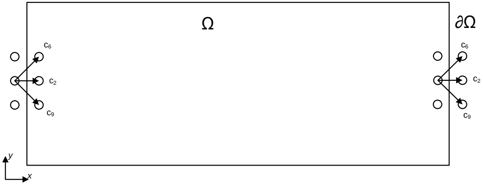
→ $\mathbf{x}$ is a fluid node if $\forall \mathbf{c}$ so that $\mathbf{x} + \mathbf{c}\Delta t \in \{\Omega \bigcup \partial\Omega\}$

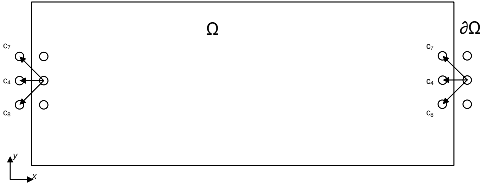
→ $\mathbf{x}$ is a boundary node if $\exists \mathbf{c}$ so that $\mathbf{x} + \mathbf{c}\Delta t \notin \{\Omega \bigcup \partial\Omega\}$



Periodic Boundary Conditions

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

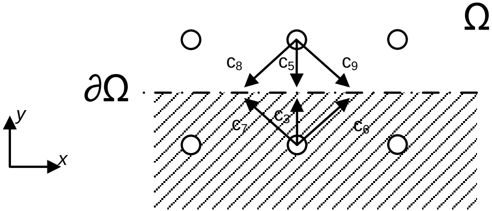




Symmetry Boundary Conditions

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

(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:

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

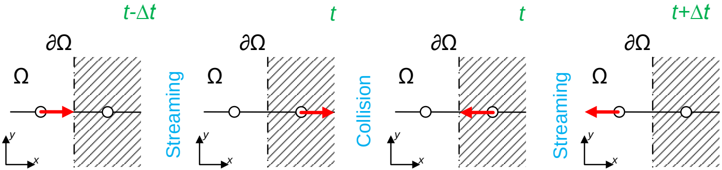
Bounceback Boundary Conditions

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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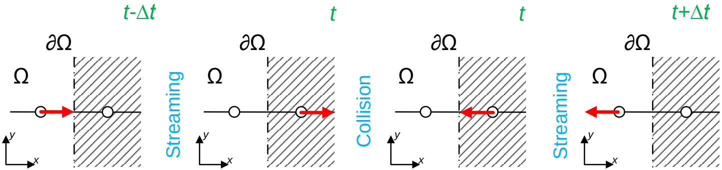
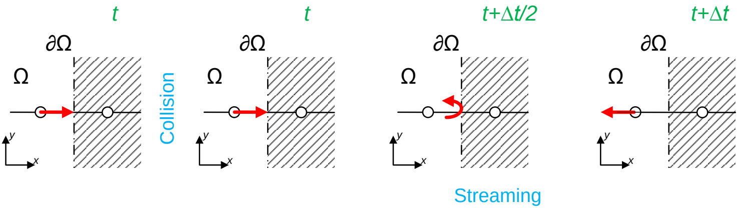
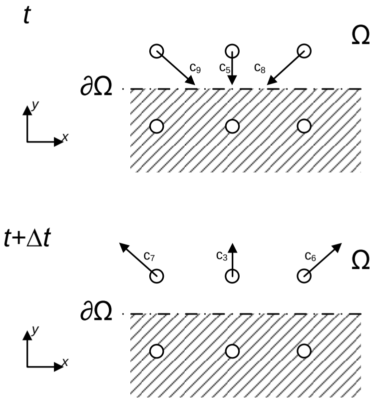


Half-way Bounceback: $f_{\bar{\alpha}}(\mathbf{x}_f, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_f, t)$



Bounceback Boundary Conditions

Half-way bounceback in 2D:



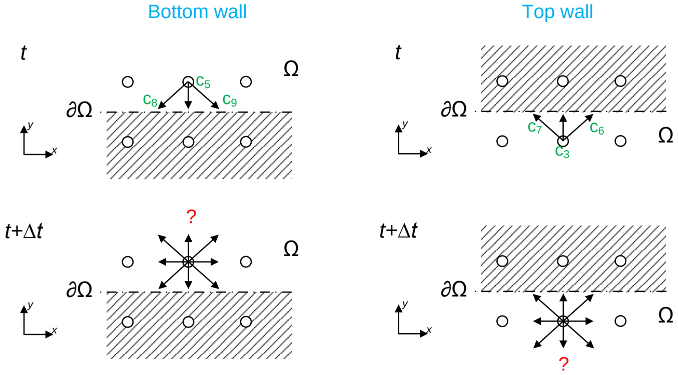
Bounceback Boundary Conditions: summary

- **Pros**
  - $\rightarrow$ Mass is exactly conserved
  - $\rightarrow$ Stable for ω close to 2 (i.e. for high Re)
  - $\rightarrow$ Local
  - $\rightarrow$ Flexibility in handling wall, edges, corners both in 2D and 3D
  - $\rightarrow$ Very simple to implement from a programming viewpoint
- **Cons**
  - $\rightarrow$ Velocity accuracy may decrease from 2^{nd} to 1^{st}
  - $\rightarrow$ Pressure accuracy may decrease from 1^{st} to 0^{th}
  - $\rightarrow$ 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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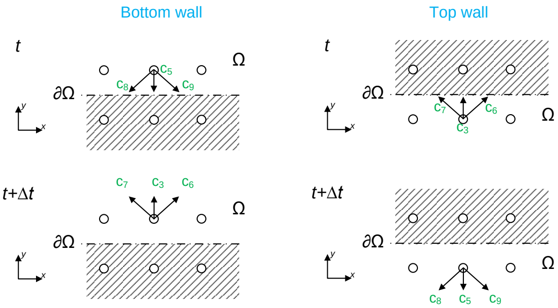

Momentum exchange

- Force (per unit volume):

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

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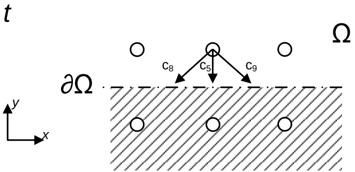

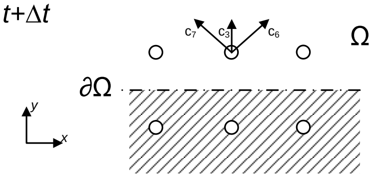

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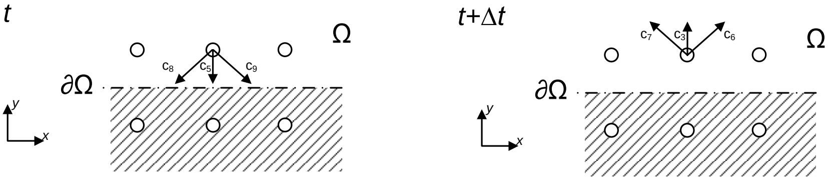

- Momentum exchange (per unit volume) between the fluid/wall surface:

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

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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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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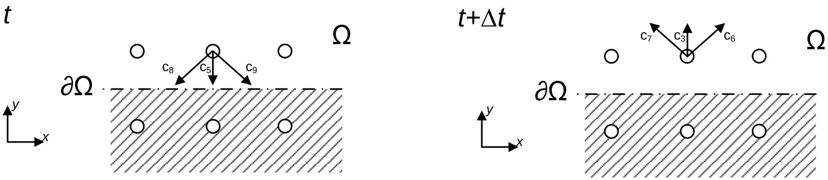

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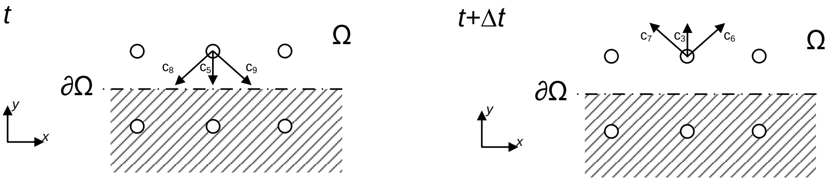

Transverse force by bottom wall:

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

Normal force on the fluid due to the bottom wall

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

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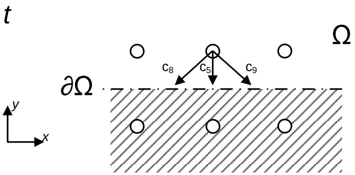
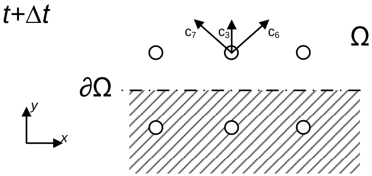
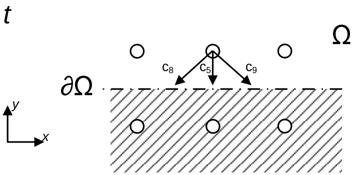
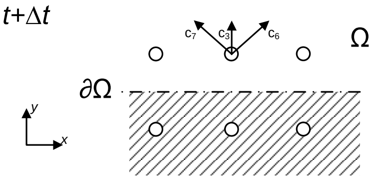




Normal force on the fluid due to the bottom wall

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





Normal force by bottom wall:

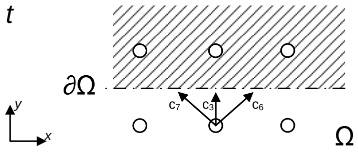
$$F_y(\mathbf{x}, t + \frac{\Delta t}{2}) = -2\frac{\Delta x}{\Delta t} \sum_{\mathbf{x}_b \in S} (\tilde{f}_5 + \tilde{f}_8 + \tilde{f}_9)|_{(\mathbf{x},t)}$$

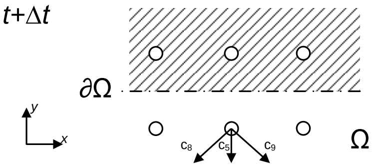
Momentum exchange: Exercise

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**:

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

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

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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:

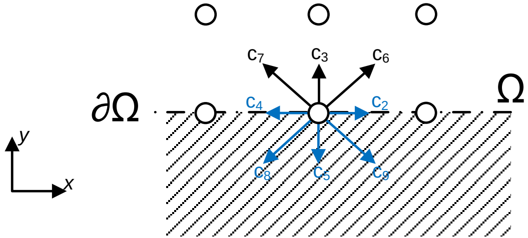
$$f_\alpha^{(0)} = w_\alpha \left(\rho + \frac{\mathbf{c}_\alpha}{c_s^2} \cdot \mathbf{u} + \frac{(\mathbf{c}_\alpha \mathbf{c}_\alpha - c_s^2 \mathbf{I})}{2 c_s^4} : \mathbf{u}\mathbf{u} \right)$$

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

Zou He boundary condition

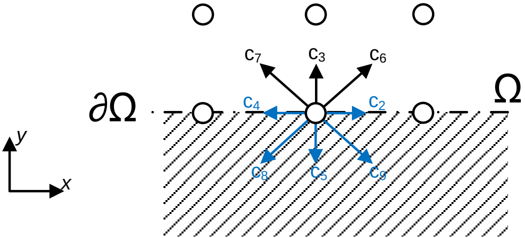
- $\rightarrow$ Boundary node and solid node coincide
- $\rightarrow$ Only unknown incoming populations are modified
- $\rightarrow$ Set ρ or $\mathbf{u}$ in $f_\alpha^{(0)}(\rho, \mathbf{u})$
- $\rightarrow$ Construct $f_\alpha^{(1)}$ from the symmetry requirement

Zou He velocity boundary condition



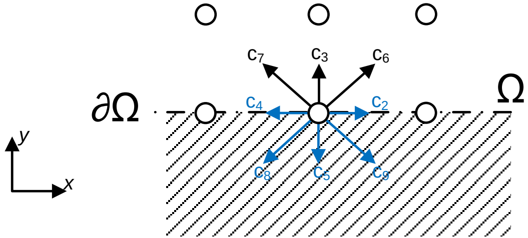
- Known:
  - $\rightarrow$ $\mathbf{u} = \mathbf{0}$
  - $\rightarrow$ $f_\alpha = (f_1, f_2, f_4, f_5, f_8, f_9)$

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:
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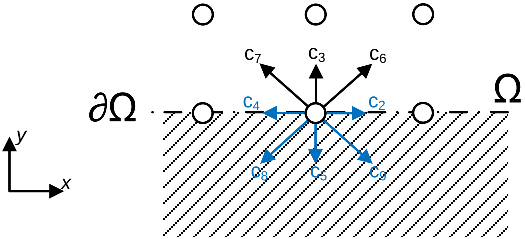
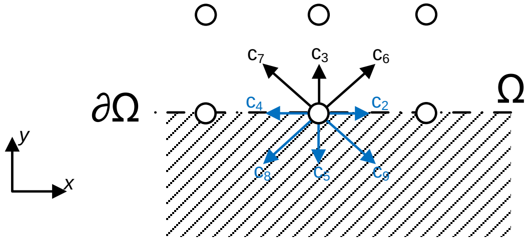
- Unknown (4 variables):
  - $\rightarrow$ ρ
  - $\rightarrow$ $f_\alpha = (f_3, f_6, f_7)$
- 3 Equations (2 linearly independent):
  - $\rightarrow$ $\sum f_\alpha = \rho$
  - $\rightarrow$ $\sum \mathbf{c}_\alpha f_\alpha = \mathbf{u}$

Zou He velocity boundary condition



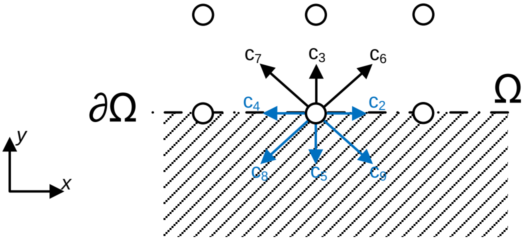
- Symmetry of $f_\alpha^{(1)}$ (3 equations):
  - $\rightarrow$ Bounceback of non-equilibrium populations

Zou He velocity boundary condition



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

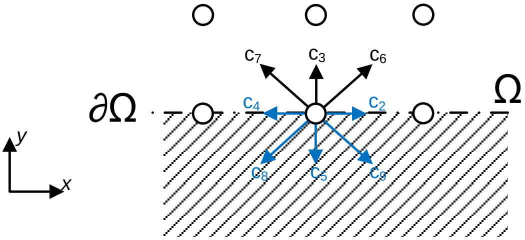
Zou He velocity boundary condition



- 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:

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

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

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

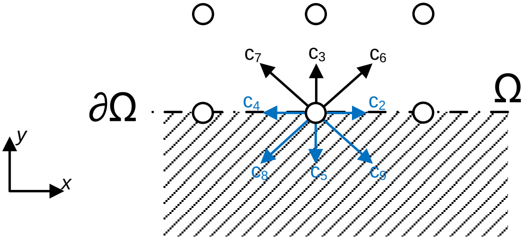
- Use the two velocity moments:

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

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

Zou He velocity boundary condition

1) Computing ρ...

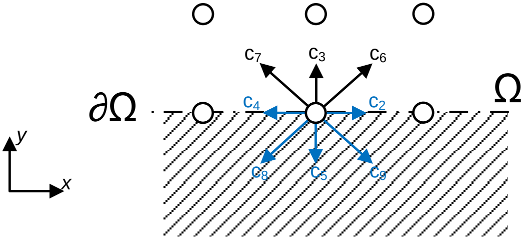


- Relate the two velocity moments:

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

Zou He velocity boundary condition

1) Computing ρ...



- Relate the two velocity moments:

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

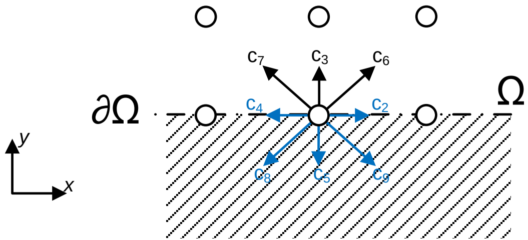
- Solution:

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

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:

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

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

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

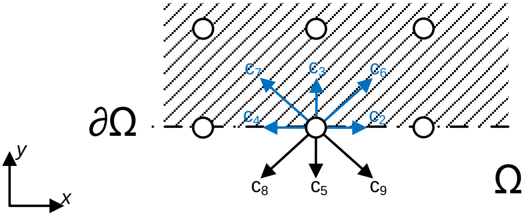
Zou He boundary condition

- **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

1. Introduction
   - Boundary Value Problems
2. Motivation
   - Navier-Stokes Boundary Conditions
3. Lattice Boltzmann Boundary Conditions
   - Problem definition
   - Boundaries in LBM
   - Particulate dynamics
   - Using Chapman-Enskog
4. Summary

Bounceback vs. Zou He

BC scheme	Bounceback	Zou He

Bounceback vs. Zou He

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Boundary location	Halfway	On node

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Viscosity independent	Not in SRT	Yes

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Viscosity independent	Not in SRT	Yes
Flexibility	Yes	Not as flexible

Bounceback vs. Zou He

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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