



UNIVERSIDADE
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LBM Workshop 2024

Boundary Conditions in lattice Boltzmann methods

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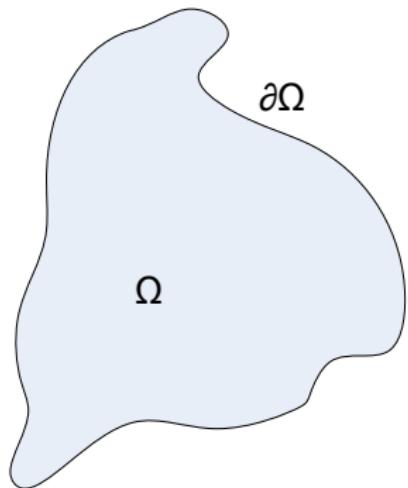
- Problem 1: Couette channel flow
- Problem 2: Poiseuille channel flow

Boundary Value Problems

- Boundary Value Problem $\left\{ \begin{array}{l} \text{Partial Differential Equation} \\ \text{Boundary Condition} \end{array} \right.$

e.g. Poisson equation for φ :

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



• Types of Boundary Conditions

→ Dirichlet Boundary Condition

$$\varphi = \varphi_b \quad \text{on } \partial\Omega$$

→ Neumann Boundary Condition

$$\mathbf{n} \cdot \nabla \varphi = \frac{\partial \varphi}{\partial n} = \varphi_b \quad \text{on } \partial\Omega$$

→ Robin Boundary Condition

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

- Steady isothermal and incompressible Navier-Stokes equations (NSEs)

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \Delta \mathbf{u} + \mathbf{a} \end{cases} \quad \text{in } \Omega$$

- Boundary Condition on solid walls

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

- Boundary Condition on fluid boundaries

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

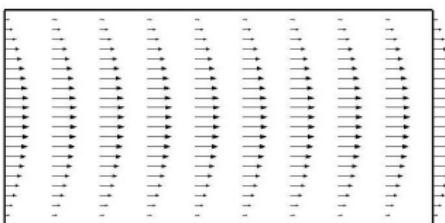
or

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

Navier-Stokes Boundary Conditions

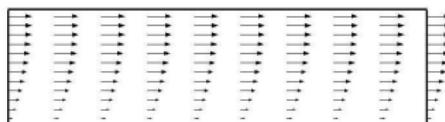
- Periodic or Cyclic Boundary Condition

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



- Symmetry Boundary Condition

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



A few things to keep in mind

LBM in a nutshell

- **Nomenclature:**

LBM = lattice Boltzmann method

- **What is LBM?**

Alternative Computational Fluid Dynamics Method

- **What are target equations of (standard) LBM?**

Isothermal Navier–Stokes Equations (NSE)

(But other extensions exist...)

- **How does LBM solves the NSE?**

Dynamics of “particles” in 2 step algorithm

Propagate along links → Equilibrate at nodes

A few things to keep in mind

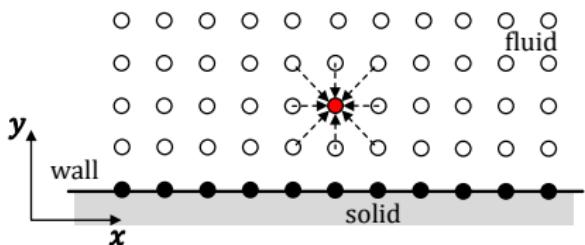
LBM is a 2 step algorithm

$$\underbrace{f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t)}_{\text{Streaming step}} = \underbrace{f_\alpha(\mathbf{x}, t) - \frac{\Delta t}{\tau} \left(f_\alpha - f_\alpha^{(\text{eq})} \right)}_{\text{Collision step}}|_{(\mathbf{x}, t)}$$

Describes *time* evolution of particles colliding and streaming in *space*

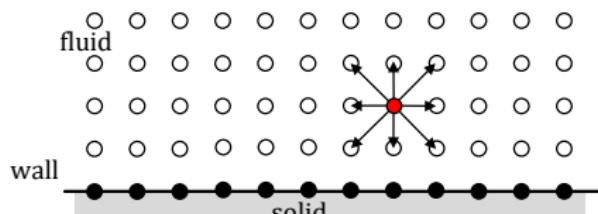
Equilibrate at nodes

(Collision step)



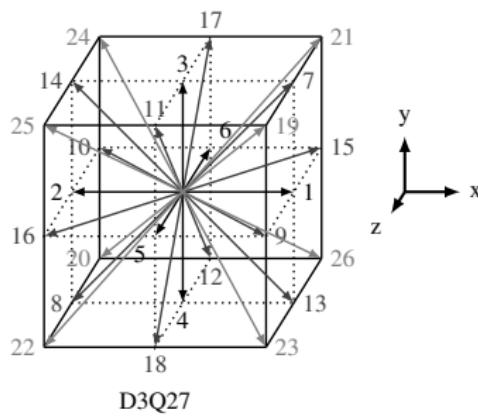
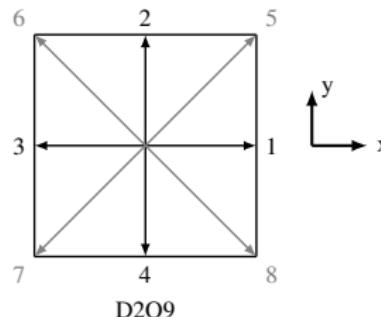
Propagate along links

(Streaming step)



A few things to keep in mind

Lattices used in LBM



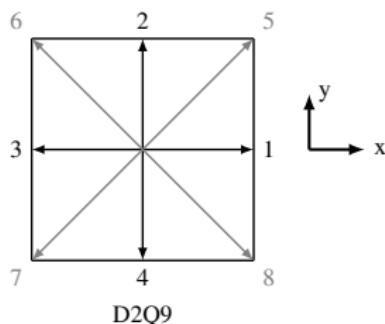
D3Q27

Lattices used in LBM



$$c_\alpha = \begin{cases} c_0 = 0 \\ c_1 = 1 \\ c_2 = -1 \end{cases}$$

D1Q3



$$\mathbf{c}_\alpha = \begin{cases} \mathbf{c}_0 = (0, 0) \\ \mathbf{c}_1 = (1, 0) \\ \mathbf{c}_2 = (0, 1) \\ \mathbf{c}_3 = (-1, 0) \\ \mathbf{c}_4 = (0, -1) \\ \mathbf{c}_5 = (1, 1) \\ \mathbf{c}_6 = (-1, 1) \\ \mathbf{c}_7 = (-1, -1) \\ \mathbf{c}_8 = (1, -1) \end{cases}$$

LBM algorithm

3. Lattice Boltzmann method algorithm

I) Initialise (Initial conditions)

Based on initial macroscopic solutions: $\rho_0 = \rho(\mathbf{x}, t = 0)$
 and $\mathbf{u}_0 = \mathbf{u}(\mathbf{x}, t = 0)$

Construct initial mesoscopic solutions

$$f_\alpha(\mathbf{x}, t = 0) = \begin{cases} f_\alpha^{(\text{eq})}(\rho_0, \mathbf{u}_0) & (\text{steady-state problems}) \\ \text{or} \\ f_\alpha^{(\text{eq})}(\rho_0, \mathbf{u}_0) + f_\alpha^{(\text{neq})}(\nabla \mathbf{u}_0, \dots) & (\text{time-dependent problems}) \end{cases}$$



II) Main algorithm

LBM algorithm

Lattice Boltzmann method algorithm

II) Main algorithm

- ① Macroscopic quantities (*local*):

$$\rho(\mathbf{x}, t) = \sum_{\alpha=0}^{Q-1} f_\alpha(\mathbf{x}, t), \quad \mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho} \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha f_\alpha(\mathbf{x}, t)$$

- ② Equilibrium (*local*):

$$f_\alpha^{(eq)}(\mathbf{x}, t) = w_\alpha \rho \left(1 + 3 \frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{c^2} + \frac{9}{2} \frac{\mathbf{c}_\alpha \mathbf{c}_\alpha : \mathbf{u} \mathbf{u}}{c^4} - \frac{3}{2} \frac{|\mathbf{u}|^2}{c^2} \right)$$

- ③ Collision (*local*):

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

- ④ Streaming (*non-local*):

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

- ⑤ Boundary conditions (*local/non-local*):

Define $f_\alpha(\mathbf{x}_{BC}, t + \Delta t) = f_\alpha(\rho_{BC}, \mathbf{u}_{BC})$ streaming out of boundary nodes

- ⑥ Test convergence? If not converged go back to step 1

LBM theory

LBM: Fully discretised Boltzmann-BGK equation

$$f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = f_\alpha(\mathbf{x}, t) - \frac{\Delta t}{\tau} (f_\alpha - f_\alpha^{(\text{eq})})|_{(\mathbf{x}, t)}$$

$$\text{with } f_\alpha^{(\text{eq})}(\mathbf{x}, t) = w_\alpha \rho \left(1 + 3 \frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{c^2} + \frac{9}{2} \frac{\mathbf{c}_\alpha \mathbf{c}_\alpha : \mathbf{u} \mathbf{u}}{c^4} - \frac{3}{2} \frac{|\mathbf{u}|^2}{c^2} \right)$$

Macroscopic quantities:

$$\text{Mass density: } \rho = \sum_{\alpha=0}^{Q-1} f_\alpha = \sum_{\alpha=0}^{Q-1} f_\alpha^{(\text{eq})}$$

$$\begin{aligned} \text{Mass density flux} &= \rho \mathbf{u} \\ \text{Momentum density: } \rho \mathbf{u} &= \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha f_\alpha = \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha f_\alpha^{(\text{eq})} \end{aligned}$$

$$\text{Momentum density flux: } \boldsymbol{\Pi} = \left(1 - \frac{\Delta t}{2\tau} \right) \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha \mathbf{c}_\alpha f_\alpha + \frac{\Delta t}{2\tau} \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha \mathbf{c}_\alpha f_\alpha^{(\text{eq})}$$

$$\text{where } \boldsymbol{\Pi}^{(\text{eq})} = \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha \mathbf{c}_\alpha f_\alpha^{(\text{eq})} = p \mathbf{I} + \rho \mathbf{u} \mathbf{u} \quad (p = c_s^2 \rho)$$

LBM theory

How does LBM approximate the macroscopic conservation laws?

Multiscale analysis: Chapman-Enskog expansion (*Advanced topic*)

- Mass balance:

$$\sum_{\alpha=0}^{Q-1} f_\alpha^{(\text{neq})} = 0 \implies \sum_{\alpha=0}^{Q-1} \epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)} + \dots = 0$$

$$(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)})\rho + \epsilon \nabla^{(1)} \cdot (\rho \mathbf{u}) = 0 \implies \boxed{\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0}$$

- Momentum balance:

$$\sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha f_\alpha^{(\text{neq})} = \mathbf{0} \implies \sum_{\alpha=0}^{Q-1} (\epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)}) \mathbf{c}_\alpha + \dots = \mathbf{0}$$

$$(\epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)}) (\rho \mathbf{u}) + \epsilon \nabla^{(1)} \cdot \left[\mathbf{\Pi}^{(\text{eq})} + \epsilon \left(1 - \frac{\Delta t}{2\tau} \right) \mathbf{\Pi}^{(1)} \right] = \mathbf{0}$$

$$\implies \boxed{\partial_t(\rho\mathbf{u}) + \nabla \cdot \left[p\mathbf{I} + \rho\mathbf{u}\mathbf{u} - \rho c_s^2 \left(\tau - \frac{\Delta t}{2} \right) (\nabla\mathbf{u} + \nabla\mathbf{u}^t + (\nabla \cdot \mathbf{u}) \mathbf{I}) \right] = \mathbf{0}}$$

Viscous shear stress $\sigma_{ij} = -\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^t + (\nabla \cdot \mathbf{u}) \mathbf{I})$ where $\mu = \rho c_s^2 (\tau - \frac{\Delta t}{2})$

LBM theory

Multiscale analysis: Chapman-Enskog expansion (*Advanced topic*)

- We have seen that at $\mathcal{O}(\epsilon^2)$ LBM is consistent with NSE
- What is accuracy of LBM as NSE solver?
 - Macroscopic equations retain a $\mathcal{O}(\epsilon^2)$ error, e.g.

$$\sum_{\alpha=0}^{Q-1} f_\alpha^{(\text{neq})} = \sum_{\alpha=0}^{Q-1} (\epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)}) = \mathcal{O}(\epsilon^3) \implies$$

$$\sum_{\alpha=0}^{Q-1} (f_\alpha^{(1)} + \epsilon f_\alpha^{(2)}) = \mathcal{O}(\epsilon^2)$$
 - Consequently, LBM approximates NSE with truncation error $\mathcal{O}(\Delta x^2)$ and $\mathcal{O}(\Delta t^2)$ (convective scaling)
- What happens at higher-orders, i.e. $\mathcal{O}(\epsilon^n)$ with $n \geq 3$?
 - At $\mathcal{O}(\epsilon^n)$ with $n \geq 3$ we obtain the truncation errors
 - Truncation errors depend on Δx and Δt (as in traditional numerical schemes) together with polynomials of τ (due to relaxation-type nature)

Multiscale analysis: Chapman-Enskog expansion (*Advanced topic*)

At steady-state:

- Dependence of spatial truncation errors on polynomials of τ :
 - $\mathcal{O}(\epsilon^3): \propto \tau(\tau^2 - \tau + \frac{1}{6})$
 - $\mathcal{O}(\epsilon^4): \propto \tau^2(\tau^2 - \tau + \frac{1}{12})$
- Given that $\nu = c_s^2 \left(\tau - \frac{\Delta t}{2} \right)$ it follows:
 - $\mathcal{O}(\epsilon^3): \propto \nu^3$
 - $\mathcal{O}(\epsilon^4): \propto \nu^4$
- Viscosity-dependent errors \implies defect of BGK collision operator

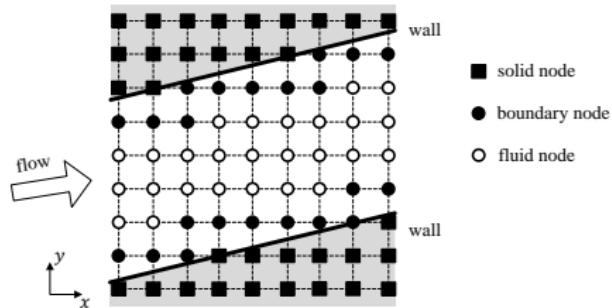
Time-dependent case is even more complicated...

Introduction

Boundary conditions in LBM

Boundary conditions apply at boundary nodes. How to identify them?

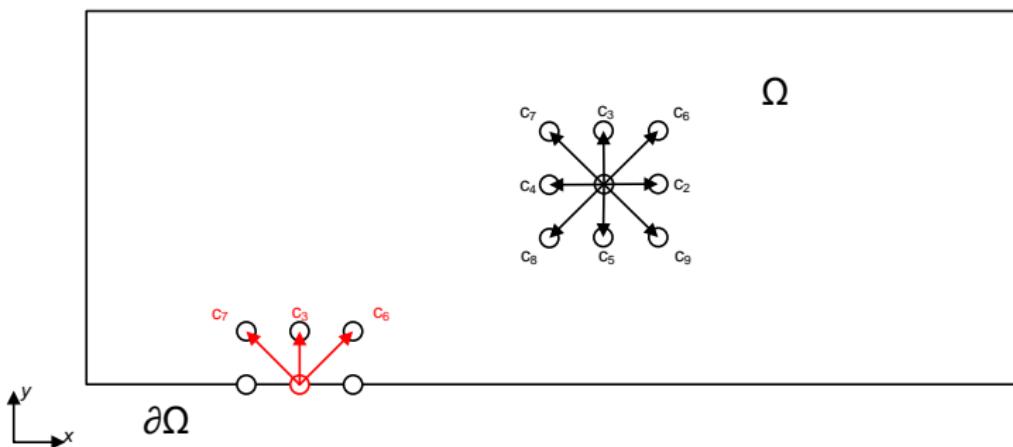
- **Fluid nodes** are sites where the LBM equation applies.
- **Solid nodes** are sites completely covered by the solid object where the LBM equation does not need to be solved.
- **Boundary nodes** link fluid and solid nodes; they require special dynamical rules to be discussed.



Introduction

Boundary conditions in LBM:

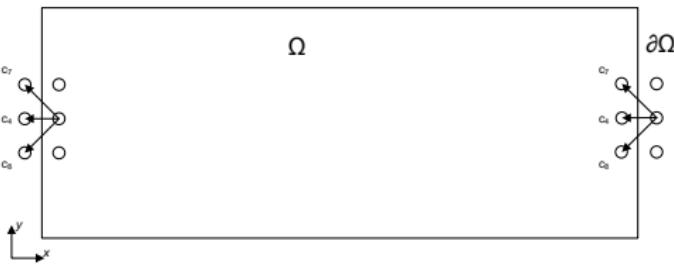
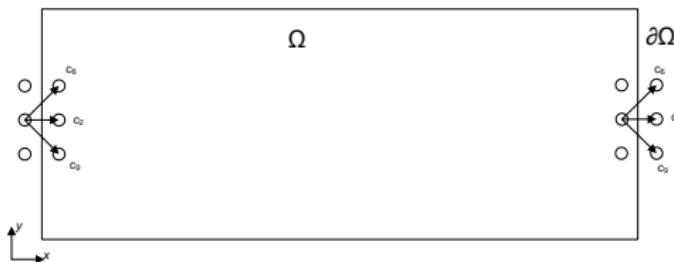
- Apply to particles that come from the **boundary nodes** into the fluid domain and cannot be determined by the streaming step.
 - The goal of the **boundary condition scheme** in LBM is to reconstruct the unknown particles that are streaming into the fluid domain from the boundary nodes.



Introduction

Example: Periodic Boundary Conditions

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



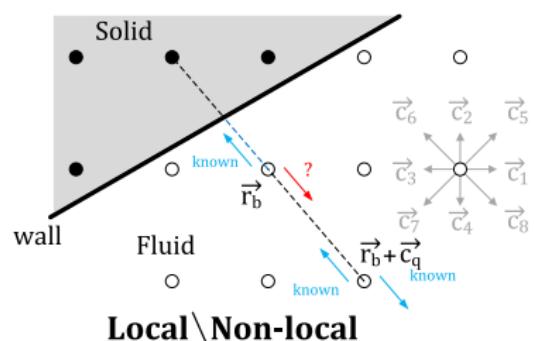
Operation principle

Challenges with boundary conditions in LBM:

- LBM operates with the particles f_α that collectively approximate the $\{\rho, \mathbf{u}, \boldsymbol{\Pi}\}$ solutions of NSEs in Ω .
- For consistency, the boundary conditions of the LBM must reproduce the intended boundary conditions of the NSEs.
- Solution on $\partial\Omega$ is specified for f_α and **NOT** for $\{\rho, \mathbf{u}, \boldsymbol{\Pi}\}$
- f_α set in a higher DoF system than $\{\rho, \mathbf{u}, \boldsymbol{\Pi}\}$, hence:
 - Trivial: $f_\alpha \rightarrow \{\rho, \mathbf{u}, \boldsymbol{\Pi}\}$
 - Complex: $\{\rho, \mathbf{u}, \boldsymbol{\Pi}\} \rightarrow f_\alpha$
- Incorrect upscaling → Unwanted behavior, e.g. unphysical velocity slip at walls, spurious Knudsen layers, etc.

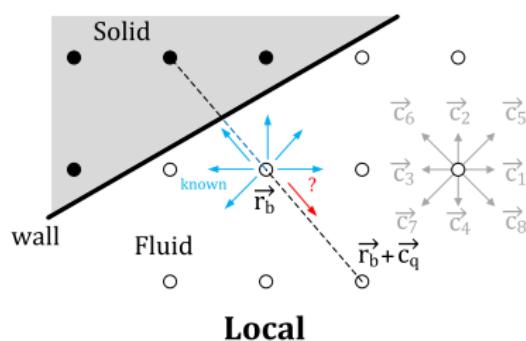
Operation principle

Two different perspectives to implement the boundary conditions in LBM

Link-wise type boundary scheme**Local\Non-local**

$$f_8(\vec{r}_b) = \mathcal{A}f_6(\vec{r}_b) + \mathcal{B}\hat{f}_8(\vec{r}_b) + \\ \mathcal{C}f_8(\vec{r}_b + \vec{c}_8) + \mathcal{D}f_6(\vec{r}_b + \vec{c}_8) + \dots$$

That is, operates along same link

Wet-node type boundary scheme**Local**

$$f_8(\vec{r}_b) = \bar{\mathcal{A}}f_1(\vec{r}_b) + \bar{\mathcal{B}}f_3(\vec{r}_b) + \\ \bar{\mathcal{C}}f_4(\vec{r}_b) + \bar{\mathcal{D}}f_5(\vec{r}_b) + \dots$$

That is, operates on same node

Boundary conditions in LBM

Link-wise family: bounce-back (BB) rule to model solid walls.

A very intuitive idea:

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

In practice, this means that:

- There is no flux crossing the wall, *i.e.* the wall is impermeable.
 - There is no relative transverse motion between fluid and wall, *i.e.* no-slip velocity at the wall.

Formulation

Boundary conditions in LBM

Recall: LBM algorithm can be operated in 2 steps.

- Collision step:

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

- Streaming step:

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

Boundary conditions in LBM

The bounce-back method can be implemented following 2 reasonings:

- **Full-way bounce-back:**

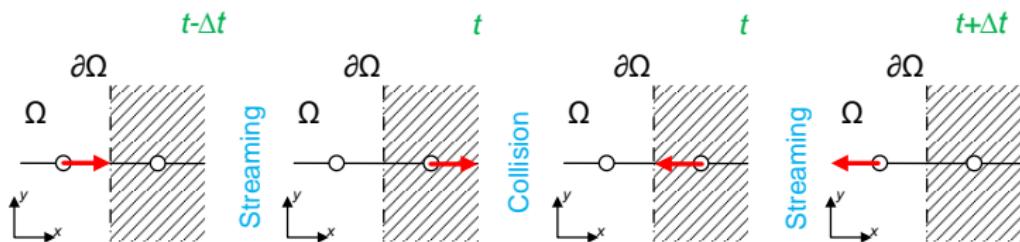
- inversion of particle velocity takes place during the **collision step**

- **Half-way bounce-back:**

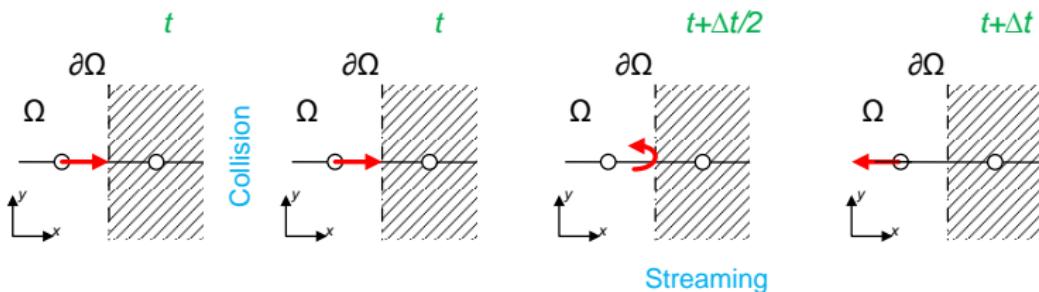
- inversion of particle velocity takes place during the **streaming step**

Boundary conditions in LBM

Full-way bounce-back: $\tilde{f}_{\bar{\alpha}}(\mathbf{x}_{\text{solid}}, t) = f_{\alpha}(\mathbf{x}_{\text{solid}}, t)$
 or $f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = f_{\alpha}(\mathbf{x}_b, t - \Delta t)$



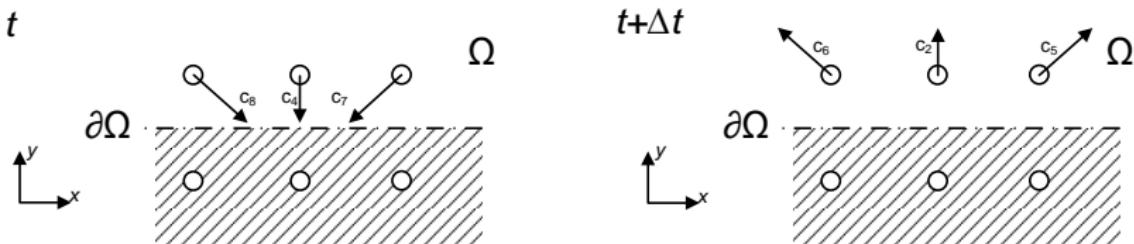
Half-way bounce-back: $f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t)$



Boundary conditions in LBM

Half-way bounce-back in 2D for horizontal bottom wall:

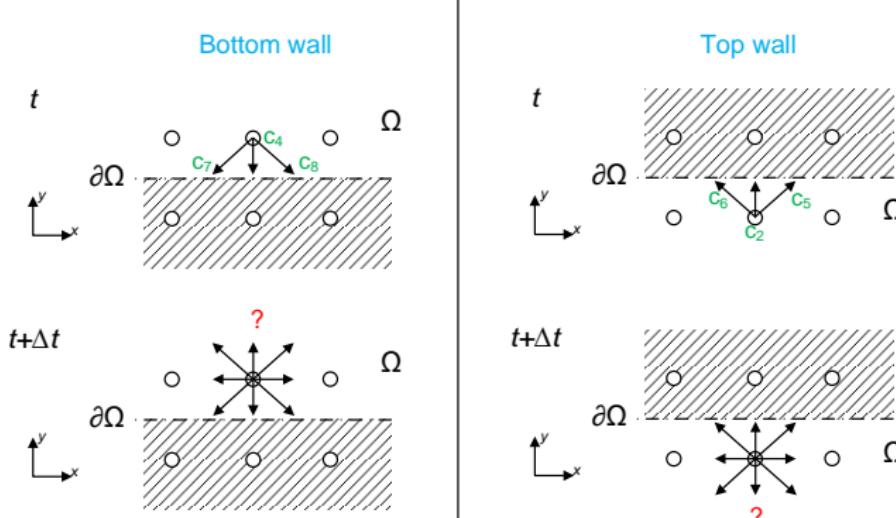
$$f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t) \quad \Rightarrow \quad \begin{cases} f_2(\mathbf{x}_b, t + \Delta t) = \tilde{f}_4(\mathbf{x}_b, t) \\ f_5(\mathbf{x}_b, t + \Delta t) = \tilde{f}_7(\mathbf{x}_b, t) \\ f_6(\mathbf{x}_b, t + \Delta t) = \tilde{f}_8(\mathbf{x}_b, t) \end{cases}$$



Bounce-back Boundary Conditions: Exercise

Question:

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

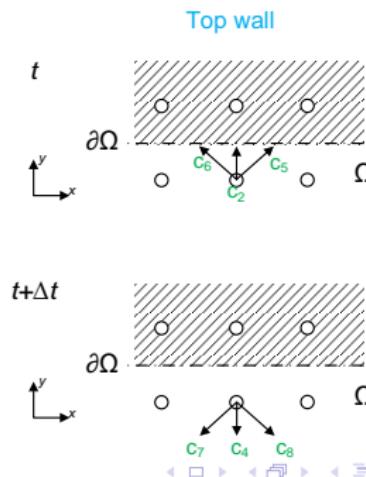
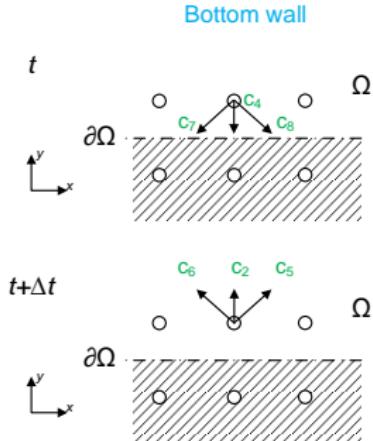


Bounce-back Boundary Conditions: Exercise

Question:

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

Solution:



Theoretical analysis

Bounce-back theoretical analysis (*Advanced topic*)Bounce-back condition for wall with arbitrary velocity \mathbf{u}_w

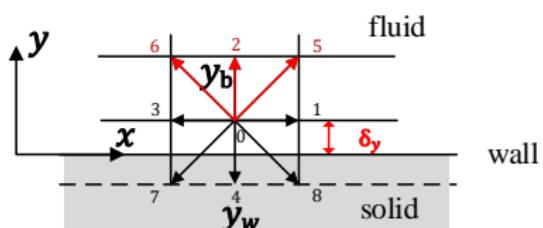
$$f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t) - 2 w_{\alpha} \rho \frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}_w}{c_s^2}$$

How does bounce-back sets the no-slip velocity condition?

Bounce-back (steady-state) closure relation
(based on Chapman-Enskog expansion)

$$\underbrace{f_{\bar{\alpha}}^{(\text{eq})} + \epsilon f_{\bar{\alpha}}^{(1)} + \epsilon^2 f_{\bar{\alpha}}^{(2)}}_{f_{\bar{\alpha}}} = \underbrace{f_{\alpha}^{(\text{eq})} + \epsilon f_{\alpha}^{(1)} + \epsilon^2 f_{\alpha}^{(2)} - \frac{\Delta}{\tau} (\epsilon f_{\alpha}^{(1)} + \epsilon^2 f_{\alpha}^{(2)}) - 2 w_{\alpha} \rho \frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}_w}{c_s^2}}_{\tilde{f}_{\alpha}}$$

Theoretical analysis

Bounce-back theoretical analysis (*Advanced topic*)

Consider a **bottom wall** located at y_w , which distances δ_y from y_b , i.e. $y_w = y_b + \delta_y$.

How does bounce-back sets the no-slip velocity condition?

Next, let us use the knowledge of $f_\alpha^{(eq)}$, $f_\alpha^{(1)}$ and $f_\alpha^{(2)}$ and neglect terms of $\mathcal{O}(u^2)$ to show that **BB sets no-slip BC as Taylor-type condition**:

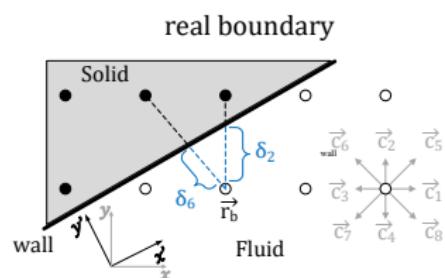
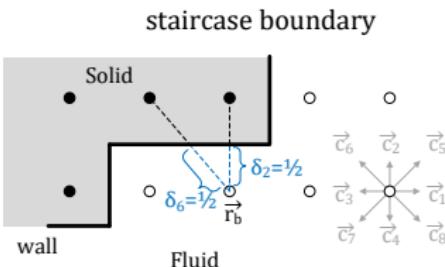
$$u_w = u_x(y_b) + \frac{\Delta x}{2} \partial_y u_x y_b + 2c_s^2 \left(\tau - \frac{\Delta t}{2}\right)^2 \partial_y^2 u_x|_{y_b}$$

If y_b is the boundary node then u_w is fulfilled $\frac{\Delta x}{2}$ away and the 2nd-order coefficient must be $\frac{\Delta x^2}{8}$. Hence, $2c_s^2 \left(\tau - \frac{\Delta t}{2}\right)^2 = \frac{\Delta x^2}{8} \xrightarrow{\nu=c_s^2(\tau-\Delta t/2)} \nu^2 = \frac{\Delta x^2}{48}$.

Theoretical analysis

Bounce-back theoretical analysis (*Advanced topic*)

BB wall:



For non mesh aligned walls the BB locates the no-slip velocity BC along the wall cut links with the accuracy:

- Error = $\mathcal{O}(\delta_\alpha^2)$ with respect to staircase wall shape
 $\Rightarrow (u_{x'} + \frac{1}{2}c_{\alpha y'} \partial_{y'} u_{x'} + \mathcal{O}(\delta_\alpha^2))(\vec{r}_b) = u_{x'}^{\text{wall}}(\vec{r}_w)$
 - Error = $\mathcal{O}(\delta_\alpha)$ with respect to real wall shape
 $\Rightarrow (u_{x'} + \mathcal{O}(\delta_\alpha))(\vec{r}_b) = u_{x'}^{\text{wall}}(\vec{x}_w)$

Boundary conditions in LBM

Wet-node boundaries: there are numerous different schemes to model solid walls. We will focus on non-equilibrium bounce-back (NEBB).

A very simple idea to understand (but not so simple to apply):

Wet boundary nodes must operate with the same dynamics as bulk nodes, i.e. they should share the same macroscopic physics of LBM in bulk.

Principle behind NEBB derivation:

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

From the Chapman-Enskog expansion:

$$f_\alpha(\mathbf{x}_w) = \underbrace{f_\alpha^{(eq)}(\rho_w, \mathbf{u}_w)}_{\text{Values at wall}} + \epsilon \underbrace{f_\alpha^{(neq)} \left(\boldsymbol{\Pi}_w^{(neq)} \propto (\nabla \mathbf{u}_w + (\nabla \mathbf{u}_w)^T) \right)}_{\text{How the wall accommodates bulk solution}}$$

Boundary conditions in LBM

Non-equilibrium bounce-back (NEBB) (also known as Zou-He method)

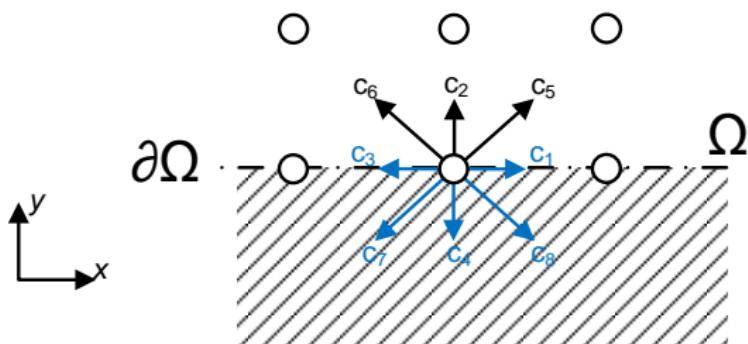
- Boundary node \mathbf{x}_b and wall node \mathbf{x}_w coincide.
- Only unknown incoming populations are modified.
- Set ρ_w and \mathbf{u}_w in $f_\alpha^{(\text{eq})}(\rho_w, \mathbf{u}_w)$ (usually \mathbf{u}_w is known but not ρ_w at walls).
- Construct $f_\alpha^{(\text{neq})}$ from symmetry requirements.

Boundary conditions in LBM

- Known:

$$\rightarrow \mathbf{u}_w = 0$$

$$\rightarrow f_q = (f_0, f_1, f_3, f_4, f_7, f_8)$$



- Unknown (4 variables):

$\rightarrow \rho_w$

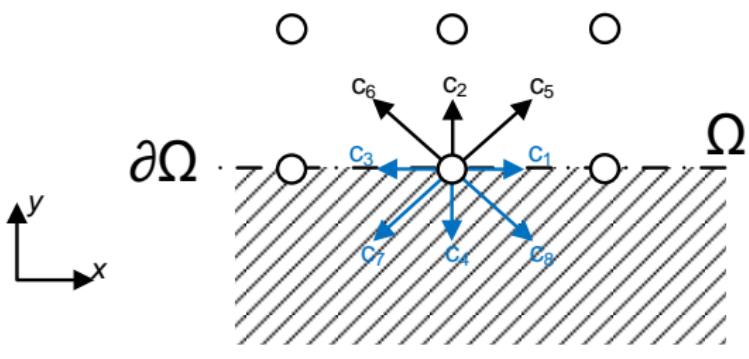
$$\rightarrow f_q = (f_2, f_5, f_6)$$

- 3 Equations (2 linearly independent):

$$\rightarrow \sum f_q = \rho_w$$

$$\rightarrow \sum \mathbf{c}_q f_q = \rho_w \mathbf{u}_w$$

Boundary conditions in LBM

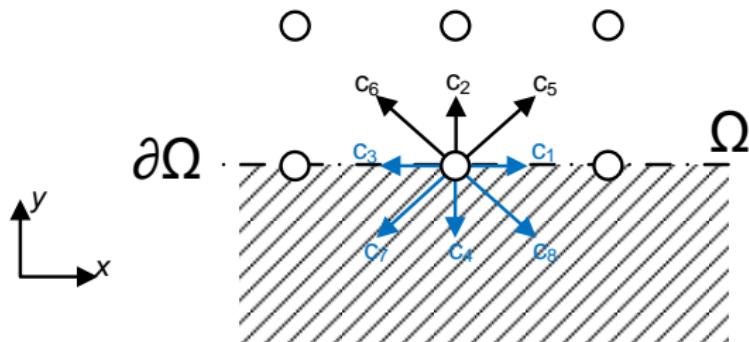


- Symmetry of $f_q^{(\text{neq})}$
(3 equations):
 - Bounce-back of non-equilibrium populations
 - Introduce extra variable (problem over-specified):
 - Transverse momentum correction N_{xy}
 - Problem is well specified:
 - 5 eqs. and 5 unknowns

Boundary conditions in LBM

1) Computing $\rho_w \dots$

- Population velocity set at boundary node:



$$\rightarrow C_+ = \{\mathbf{c}_2, \mathbf{c}_5, \mathbf{c}_6\}$$

$$\rightarrow C_0 = \{\mathbf{c}_0, \mathbf{c}_1, \mathbf{c}_3\}$$

$$\rightarrow C_- = \{\mathbf{c}_4, \mathbf{c}_7, \mathbf{c}_8\}$$

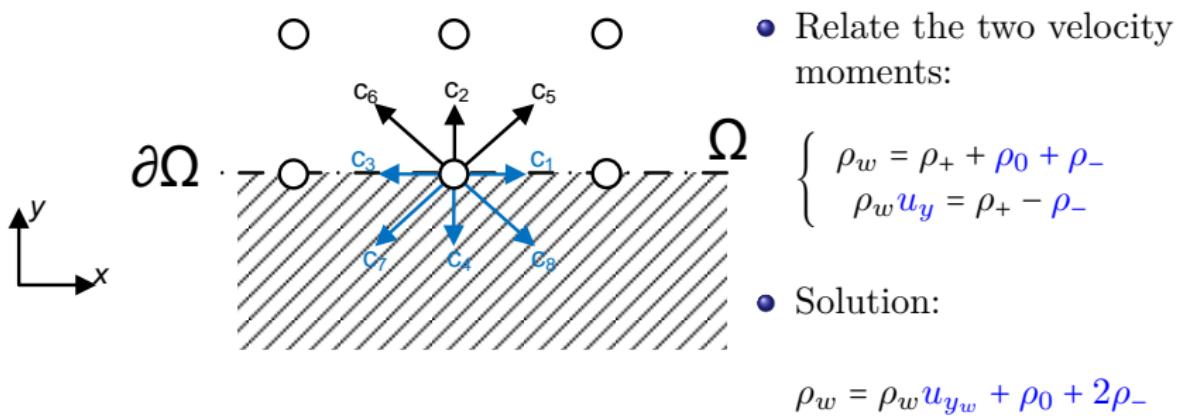
- Use the two velocity moments:

$$\rightarrow \sum f_q = \rho$$

$$\rightarrow \sum c_{qy} f_q = \rho u_y$$

Boundary conditions in LBM

1) Computing ρ_w ...

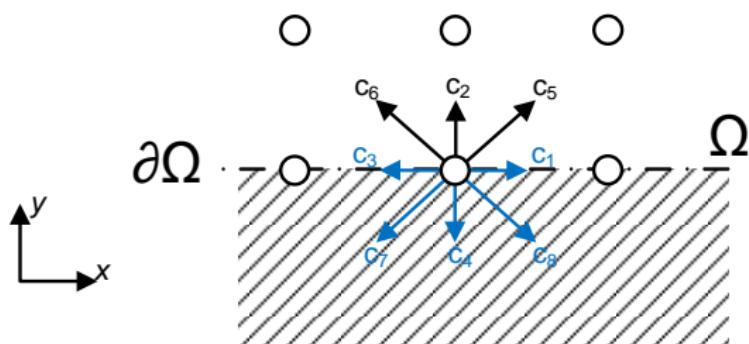


$$\text{i.e. } \rho_w = \rho_w u_{y_w} + (f_0 + f_1 + f_3) + 2(f_4 + f_7 + f_8)$$

$$\Rightarrow \quad \rho_w = \frac{1}{1-u_{y_w}} \left((f_0 + f_1 + f_3) + 2(f_4 + f_7 + f_8) \right)$$

Boundary conditions in LBM

2) Computing $\{f_2, f_5, f_6\}\dots$



- Non-equilibrium bounce-back with transverse momentum correction:

$$f_2 - f_2^{(0)} = f_4 - f_4^{(0)}$$

$$f_5 - f_5^{(0)} = f_7 - f_7^{(0)} + N_{xy}$$

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

Boundary conditions in LBM

2) Computing $\{f_2, f_5, f_6\} \dots$

Solution for the unknown incoming populations:

$$f_2 = f_4 + \frac{2}{3}\rho_w u_{y_w}$$

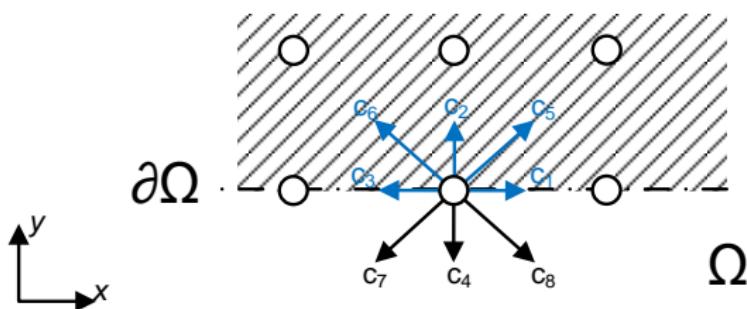
$$f_5 = f_7 + \frac{1}{2}(f_3 - f_1) + \frac{1}{6}\rho_w u_{y_w} + \frac{1}{2}\rho_w u_{x_w}$$

$$f_6 = f_8 - \frac{1}{2}(f_3 - f_1) + \frac{1}{6}\rho_w u_{y_w} - \frac{1}{2}\rho_w u_{x_w}$$

NEBB boundary condition: Exercise

Question:

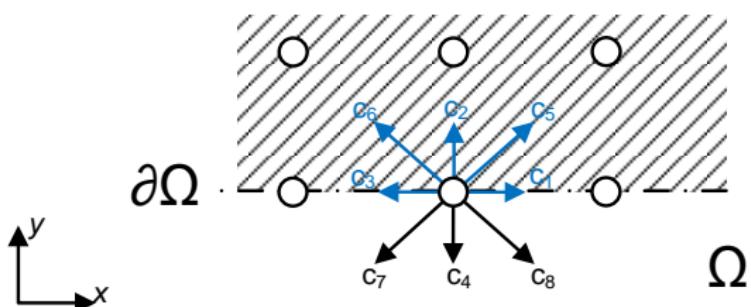
Use the Non-equilibrium bounce-back (NEBB) rule to find the unknown ρ and the unknown populations at the top wall



Question: Boundary conditions in LBM

1) Computing ρ_w ...

- Population velocity set at boundary node:



$$\rightarrow C_+ = \{c_2, c_5, c_6\}$$

$$\rightarrow C_0 = \{c_0, c_1, c_3\}$$

$$\rightarrow C_- = \{c_4, c_7, c_8\}$$

- Solution:

$$\rho_w = -\rho_w u_{y_w} + \rho_0 + 2\rho_+$$

$$\text{i.e. } \rho_w = -\rho_w u_{y_w} + (f_0 + f_1 + f_3) + 2(f_2 + f_5 + f_6)$$

$$\Rightarrow \rho_w = \frac{1}{1+u_{y_w}} \left((f_0 + f_1 + f_3) + 2(f_2 + f_5 + f_6) \right)$$

NEBB boundary condition: Exercise

Question: Boundary conditions in LBM

2) Computing $\{f_4, f_7, f_8\} \dots$

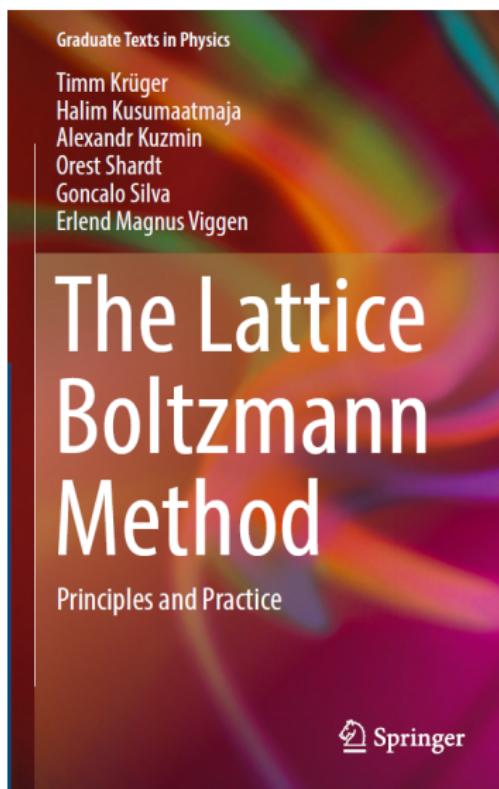
Solution for the unknown incoming populations:

$$f_4 = f_2 - \frac{2}{3}\rho_w u_{y_w}$$

$$f_7 = f_5 - \frac{1}{2}(f_3 - f_1) - \frac{1}{6}\rho_w u_{y_w} - \frac{1}{2}\rho_w u_{x_w}$$

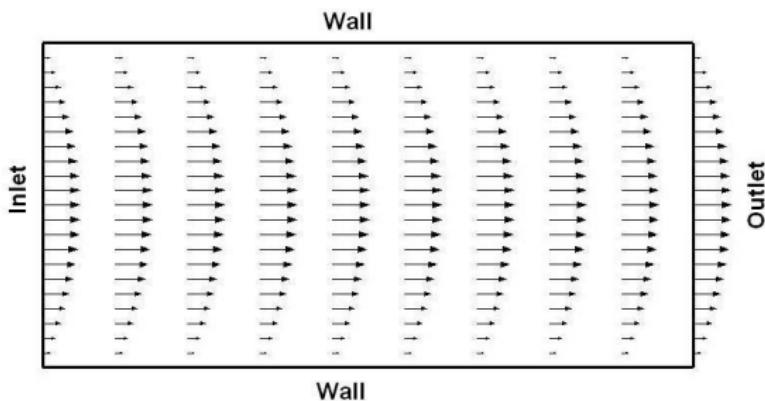
$$f_8 = f_6 + \frac{1}{2}(f_3 - f_1) - \frac{1}{6}\rho_w u_{y_w} + \frac{1}{2}\rho_w u_{x_w}$$

Thank you for your attention.



Numerical Lab

Testing the LBM for different BC schemes

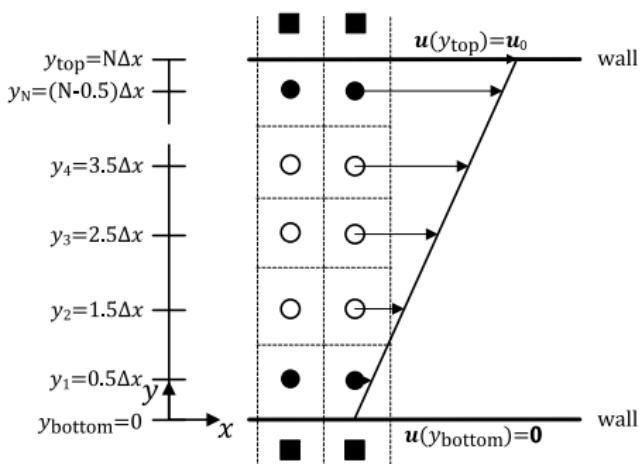
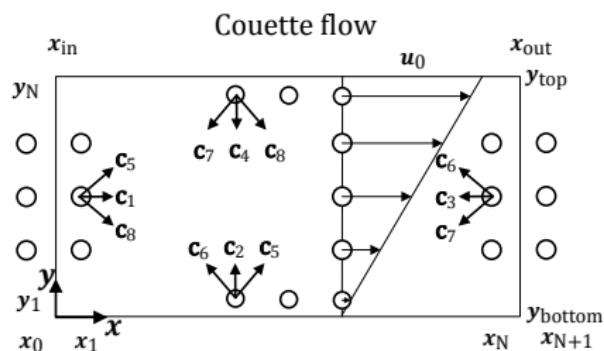


Problem 1: Couette channel flow

Exercise I:

Couette flow in channel with BB boundaries

Walls midway grid nodes



- Analytical solution: $u_x = u_0 \frac{y_j}{L_y}$.
- Reynolds number: $\text{Re} = \frac{u_0 L_y}{\nu}$ where $L_y = N_y \Delta x$.
- Bounce-back walls:** $y_j = -\frac{\Delta x}{2} + j \Delta x$ where $j = 1, 2, \dots, N_y$.

Problem 1: Couette channel flow

Input parameters

- N_{steps} → Number of time steps to achieve steady-state
- N_x → Number of nodes along the channel length
- N_y → Number of nodes along the channel height
- Re → Flow Reynolds number

and

- U_{max} → Maximum velocity (proportional to Mach number)
- or τ → Relaxation time (LBM parameter)

Problem 1: Couette channel flow

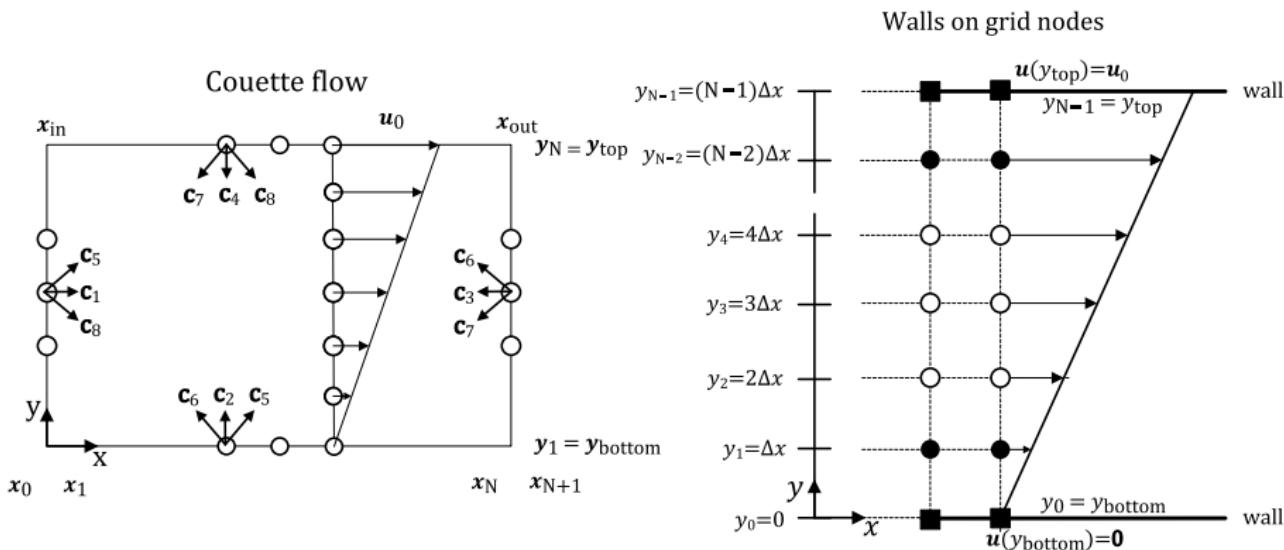
Couette flow in channel with BB boundaries

- **Question 1:** Fix $Re = 10$ and $U_{max} = 0.1$
 - **Question 1.1** For $N_y = 16$, what is τ and $\|L_2\|$ error norm?
 - **Question 1.2** For $N_y = 32$, what is τ and $\|L_2\|$ error norm?
 - **Question 1.3** Does error decrease with mesh resolution?
- **Question 2:** Repeat the analysis, changing to $Re = 0.1$

Problem 1: Couette channel flow

Exercise II:

Couette flow in channel with NEBB boundaries



- Analytical solution: $u_x = u_0 \frac{y_j}{L_y}$.
- Reynolds number: $Re = \frac{u_0 L_y}{\nu}$ where $L_y = (N_y - 1) \Delta x$.
- NEBB walls:** $y_j = (j - 1) \Delta x$ where $j = 1, 2, \dots, N_y$.

Problem 1: Couette channel flow

Couette flow in channel with NEBB boundaries

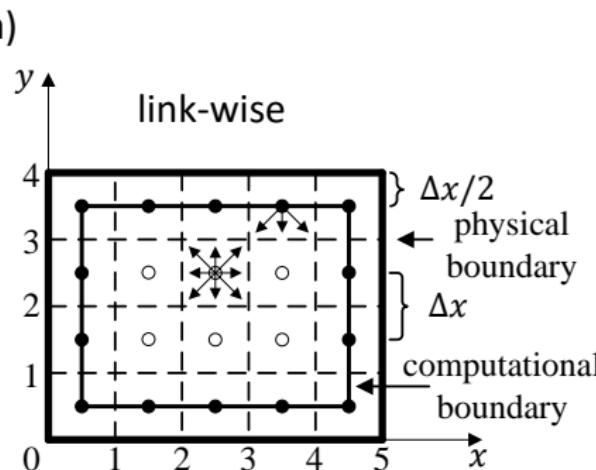
- **Question 1:** Fix $Re = 10$ and $U_{max} = 0.1$
 - **Question 1.1** For $N_y = 16$, what is τ and $\|L_2\|$ error norm?
 - **Question 1.2** For $N_y = 32$, what is τ and $\|L_2\|$ error norm?
 - **Question 1.3** Does error decrease with mesh resolution?
- **Question 2:** Repeat the analysis, changing to $Re = 0.1$

Problem 1: Couette channel flow

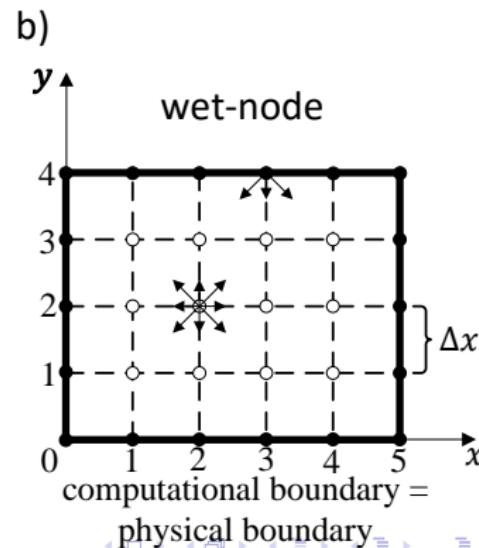
Conclusion: Boundary conditions apply at boundary nodes, which may or may not coincide with the boundaries of the physical domain.

Question: Where are grid nodes located in computational cells?

a) Grid nodes are cell centred



b) Grid nodes are vertex centred

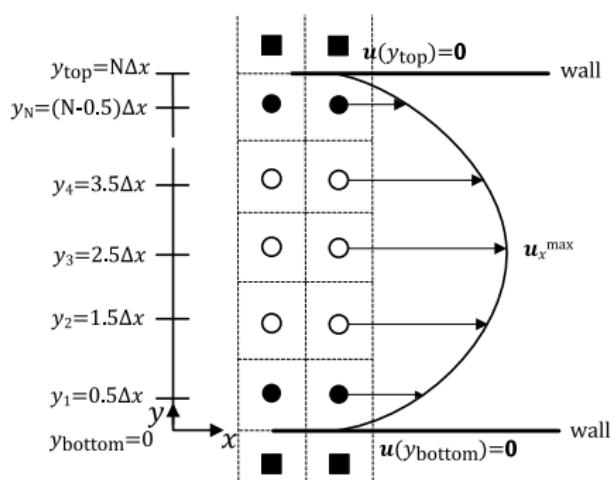
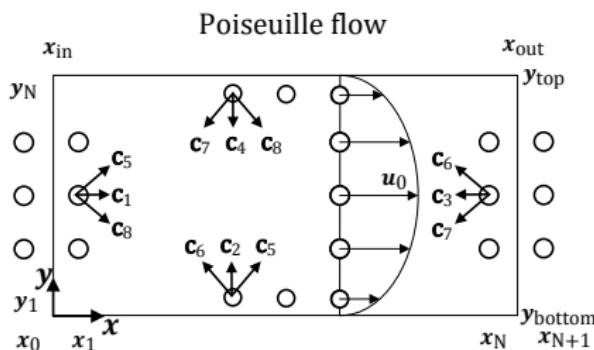


Problem 2: Poiseuille channel flow

Exercise III:

Poiseuille flow in channel with BB boundaries

Walls midway grid nodes



- Analytical solution: $u_x = -\frac{4}{L_y^2} u_0 y_j (y_j - L_y)$ where $u_0 = \frac{F_x L_y^2}{8 \nu}$.
- Reynolds number: $Re = \frac{u_0 L_y}{\nu}$ where $L_y = N_y \Delta x$.
- Bounce-back walls:** $y_j = -\frac{\Delta x}{2} + j \Delta x$ where $j = 1, 2, \dots, N_y$.

Problem 2: Poiseuille channel flow

Poiseuille flow in channel with BB boundaries

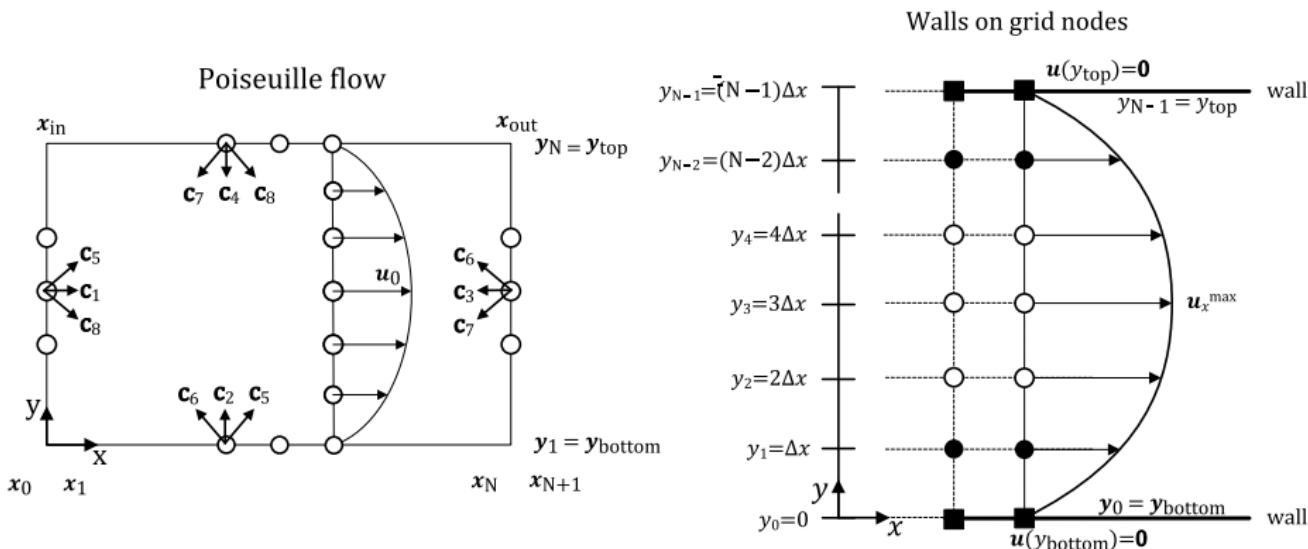
- **Question 1:** Fix $Re = 10$ and $\tau = 0.9$
 - **Question 1.1** For $N_y = 16$, what is U_{max} and $\|L_2\|$ error norm?
 - **Question 1.2** For $N_y = 32$, what is U_{max} and $\|L_2\|$ error norm?
 - **Question 1.3** Estimate the convergence rate

Hint: $\alpha = \ln\left(\frac{\|L_2\|_\infty(u_{2N})}{\|L_2\|_\infty(u_N)}\right)/\ln\left(\frac{2N}{N}\right)$

- **Question 2:** Repeat the analysis, changing to $\tau = \sqrt{\frac{3}{16}} + \frac{1}{2}$

Exercise III:

Poiseuille flow in channel with NEBB boundaries



- Analytical solution: $u_x = -\frac{4 u_0}{L_y^2} y_j (y_j - L_y)$ where $u_0 = \frac{F_x L_y^2}{8 \nu}$.

- Reynolds number: $Re = \frac{u_0 L_y}{\nu}$ where $L_y = N_y \Delta x$.

- Bounce-back walls:** $y_j = (j - 1) \Delta x$ where $j = 1, 2, \dots, N_y$.

Problem 2: Poiseuille channel flow

Poiseuille flow in channel with NEBB boundaries

- **Question 1:** Fix $Re = 10$ and $\tau = 0.9$
 - **Question 1.1** For $N_y = 16$, what is U_{max} and $\|L_2\|$ error norm?
 - **Question 1.2** For $N_y = 32$, what is U_{max} and $\|L_2\|$ error norm?
 - **Question 1.3** Does the error decrease with mesh resolution?
- **Question 2:** Repeat the analysis for other τ values