LBM Workshop 2024
Boundary Conditions in lattice Boltzmann methods

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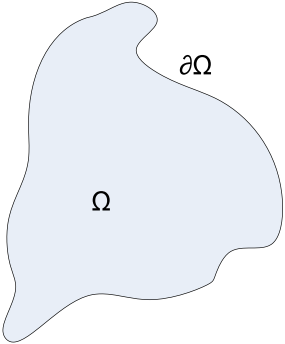
Boundary Value Problems

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

e.g. Poisson equation for φ:

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



- 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)**

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

- Boundary Condition on solid walls

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

- Boundary Condition on fluid boundaries

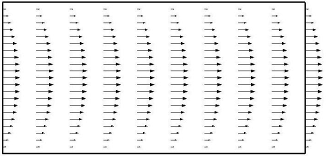
$$\mathbf{u} = \mathbf{u}_{in} \quad \text{on } \partial\Omega$$

or

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

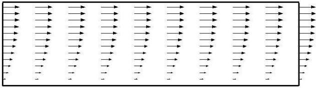
- Periodic or Cyclic Boundary Condition

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



- Symmetry Boundary Condition

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



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

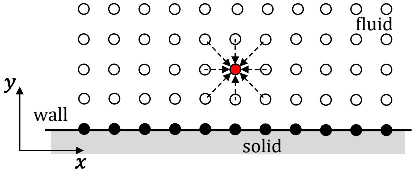
LBM is a 2 step algorithm

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

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

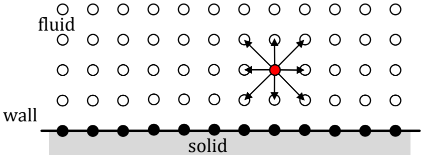
Equilibrate at nodes

(Collision step)

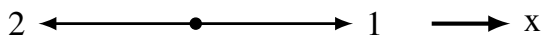


Propagate along links

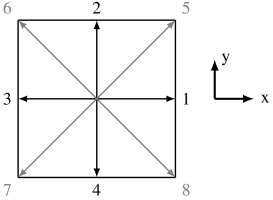
(Streaming step)



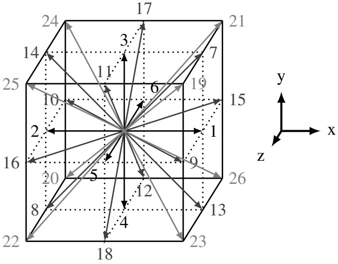
Lattices used in LBM



D1Q3

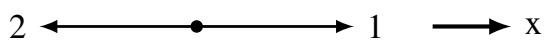


D2Q9



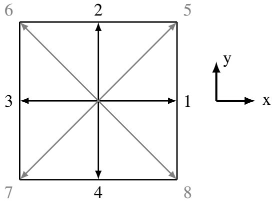
D3Q27

Lattices used in LBM



D1Q3

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



D2Q9

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

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

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

$$\Downarrow$$

II) Main algorithm

Lattice Boltzmann method algorithm

II) Main algorithm

1. Macroscopic quantities (*local*):
$$\boxed{\rho(\mathbf{x},t) = \sum_{\alpha=0}^{Q-1} f_\alpha(\mathbf{x},t), \quad \mathbf{u}(\mathbf{x},t) = \frac{1}{\rho}\sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha f_\alpha(\mathbf{x},t)}$$
2. Equilibrium (*local*): $\boxed{f_\alpha^{(\mathrm{eq})}(\mathbf{x},t) = w_\alpha \rho \left(1 + 3\,\frac{\mathbf{c}_\alpha \cdot \mathbf{u}}{c^2} + \frac{9}{2}\,\frac{\mathbf{c}_\alpha \mathbf{c}_\alpha : \mathbf{u}\mathbf{u}}{c^4} - \frac{3}{2}\,\frac{|\mathbf{u}|^2}{c^2}\right)}$
3. Collision (*local*): $\boxed{\tilde{f}_\alpha(\mathbf{x},t) = f_\alpha(\mathbf{x},t) - \frac{\Delta t}{\tau}\left(f_\alpha - f_\alpha^{(\mathrm{eq})}\right)\big|_{(\mathbf{x},t)}}$
4. Streaming (*non-local*): $\boxed{f_\alpha(\mathbf{x} + \mathbf{c}_\alpha \Delta t, t + \Delta t) = \tilde{f}_\alpha(\mathbf{x},t)}$
5. Boundary conditions (*local*/*non-local*):
Define $\boxed{f_\alpha(\mathbf{x}_{\mathrm{BC}}, t + \Delta t) = f_\alpha(\rho_{\mathrm{BC}}, \mathbf{u}_{\mathrm{BC}})}$ streaming out of boundary nodes
6. Test convergence? If not converged go back to step 1

LBM: Fully discretised Boltzmann-BGK equation

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

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

Macroscopic quantities:

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

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

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

where $$\mathbf{\Pi}^{(\mathrm{eq})} = \sum_{\alpha=0}^{Q-1} \mathbf{c}_\alpha\mathbf{c}_\alpha f_\alpha^{(\mathrm{eq})} = p\,\mathbf{I} + \rho\mathbf{uu} \qquad (p = c_s^2\rho)$$

How does LBM approximate the macroscopic conservation laws?

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

- **Mass balance:**

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

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

- **Momentum balance:**

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

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

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

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

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. $\sum_{\alpha=0}^{Q-1} f_\alpha^{(\mathrm{neq})} = \sum_{\alpha=0}^{Q-1}(\epsilon f_\alpha^{(1)} + \epsilon^2 f_\alpha^{(2)}) = \mathcal{O}(\epsilon^3) \Longrightarrow \sum_{\alpha=0}^{Q-1}(f_\alpha^{(1)} + \epsilon f_\alpha^{(2)}) = \mathcal{O}(\epsilon^2)$
  - 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:
  - $\mathcal{O}(\epsilon^3)$: $\propto \nu^3$
  - $\mathcal{O}(\epsilon^4)$: $\propto \nu^4$

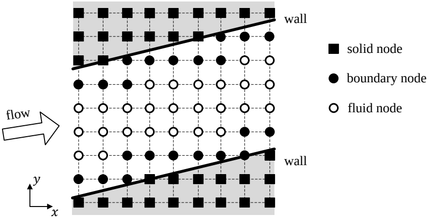
- Viscosity-dependent errors $\Longrightarrow$ defect of BGK collision operator

Time-dependent case is even more complicated...

Boundary conditions in LBM

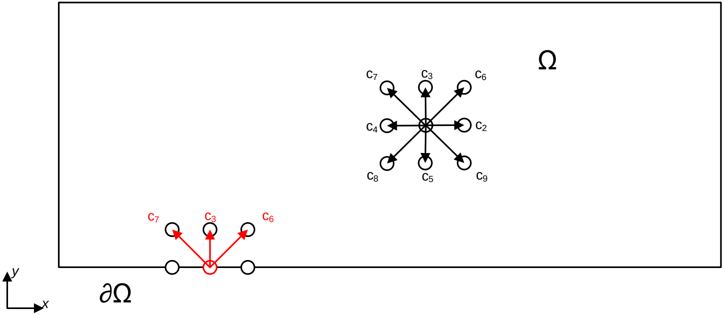
Boundary conditions apply at boundary nodes. How to identify them?

- **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.



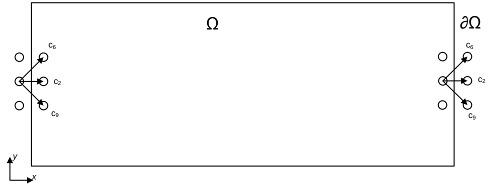
Boundary conditions in LBM:

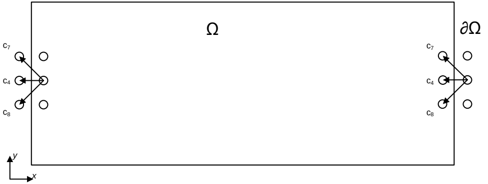
- Apply to particles that come from the **boundary nodes** into the fluid domain and cannot be determined by the streaming step.
- The goal of the **boundary condition scheme in LBM** is to reconstruct the unknown particles that are streaming into the fluid domain from the boundary nodes.



Example: Periodic Boundary Conditions

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



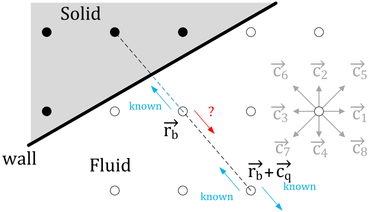


Challenges with boundary conditions in LBM:

- → LBM operates with the particles f_α that collectively approximate the $\{\rho, \mathbf{u}, \mathbf{\Pi}\}$ 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 $\{\rho, \mathbf{u}, \mathbf{\Pi}\}$
- → 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: $\{\rho, \mathbf{u}, \mathbf{\Pi}\} \longrightarrow f_\alpha$
- → Incorrect upscaling $\longrightarrow$ Unwanted behavior, e.g. unphysical velocity slip at walls, spurious Knudsen layers, etc.

Two different perspectives to implement the boundary conditions in LBM

Link-wise type boundary scheme

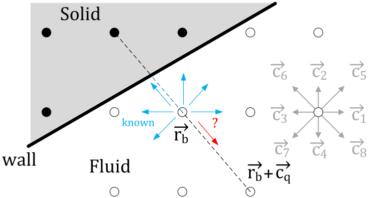


Local\Non-local

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

That is, operates along same link

Wet-node type boundary scheme



Local

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

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.

Boundary conditions in LBM

Recall: LBM algorithm can be operated in 2 steps.

- Collision step:

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

- Streaming step:

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

Boundary conditions in LBM

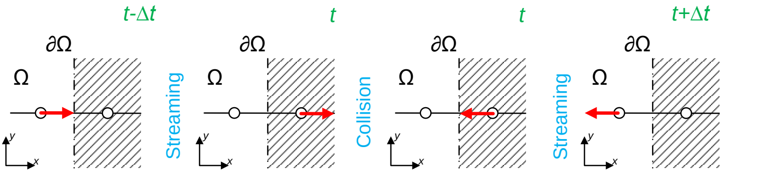
The bounce-back method can be implemented following 2 reasonings:

- **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**

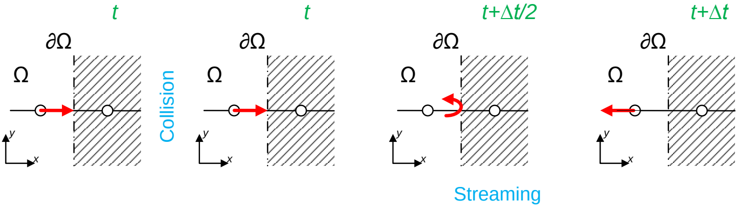
Boundary conditions in LBM

Full-way bounce-back: $\tilde{f}_{\bar{\alpha}}(\mathbf{x}_{\mathrm{solid}}, t) = \tilde{f}_{\alpha}(\mathbf{x}_{\mathrm{solid}}, t)$

or $\quad f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = f_{\alpha}(\mathbf{x}_b, t - \Delta t)$



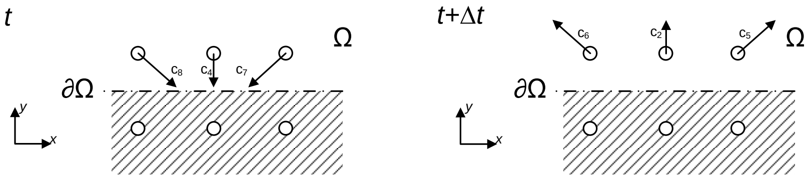
Half-way bounce-back: $f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t)$



Boundary conditions in LBM

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

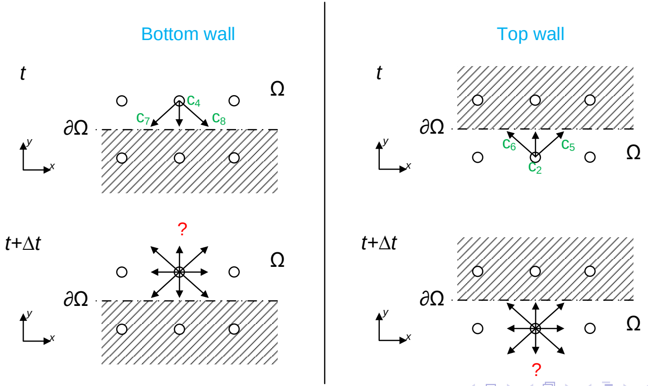
$$f_{\bar{\alpha}}(\mathbf{x}_b, t+\Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t) \quad \Rightarrow \quad \begin{cases} f_2(\mathbf{x}_b, t+\Delta t) = \tilde{f}_4(\mathbf{x}_b, t) \\ f_5(\mathbf{x}_b, t+\Delta t) = \tilde{f}_7(\mathbf{x}_b, t) \\ f_6(\mathbf{x}_b, t+\Delta t) = \tilde{f}_8(\mathbf{x}_b,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



Bounce-back Boundary Conditions: Exercise

Question:

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

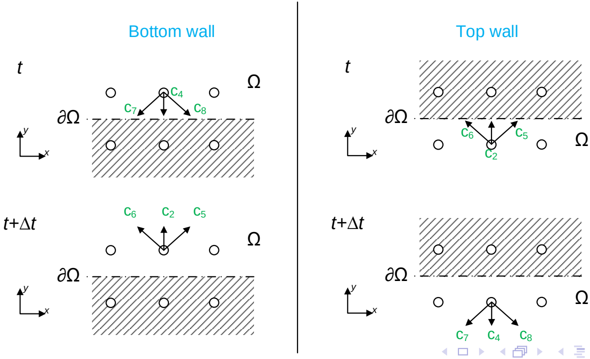


Bounce-back Boundary Conditions: Exercise

Question:

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

Solution:



Bounce-back theoretical analysis (*Advanced topic*)

Bounce-back condition for wall with arbitrary velocity $\mathbf{u}_w$

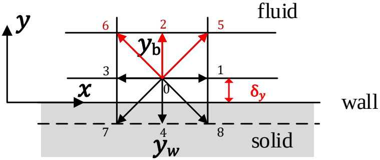
$$f_{\bar{\alpha}}(\mathbf{x}_b, t + \Delta t) = \tilde{f}_{\alpha}(\mathbf{x}_b, t) - 2\, w_{\alpha}\, \rho\, \frac{\mathbf{c}_{\alpha} \cdot \mathbf{u}_w}{c_s^2}$$

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

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

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

Bounce-back theoretical analysis (*Advanced topic*)



Consider a **bottom wall** located at y_{w}, which distances δ_y from y_b, i.e. $y_{\mathrm{w}} = y_b + \delta_y$.

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

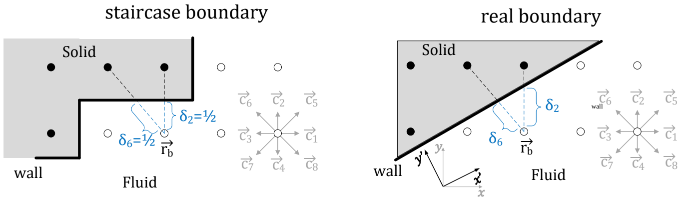
Next, let us use the knowledge of $f_\alpha^{(\mathrm{eq})}$, $f_\alpha^{(1)}$ and $f_\alpha^{(2)}$ and neglect terms of $\mathcal{O}(u^2)$ to show that **BB sets no-slip BC as Taylor-type condition**:

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

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

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

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:

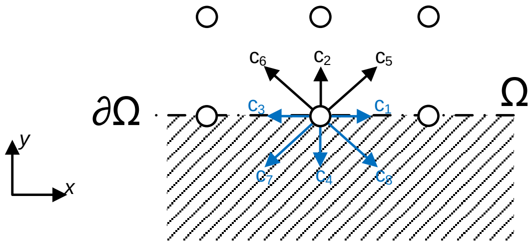
$$f_\alpha(\mathbf{x}_w) = \underbrace{f_\alpha^{(\mathrm{eq})}(\rho_w, \mathbf{u}_w)}_{\text{Values at wall}} + \underbrace{\epsilon\, f_\alpha^{(\mathrm{neq})}\left(\mathbf{\Pi}_w^{(\mathrm{neq})} \propto \left(\nabla \mathbf{u}_w + (\nabla \mathbf{u}_w)^T\right)\right)}_{\text{How the wall accommodates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

Boundary conditions in LBM

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

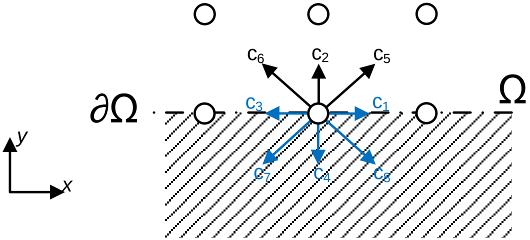
- Boundary node $\mathbf{x}_b$ and wall node $\mathbf{x}_w$ coincide.
- Only unknown incoming populations are modified.
- Set ρ_w and $\mathbf{u}_w$ in $f_\alpha^{(\mathrm{eq})}(\rho_w, \mathbf{u}_w)$ (usually $\mathbf{u}_w$ is known but not ρ_w at walls).
- Construct $f_\alpha^{(\mathrm{neq})}$ from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

Boundary conditions in LBM



- Known:
  - → $\mathbf{u}_w = \mathbf{0}$
  - → $f_q = (f_0, f_1, f_3, f_4, f_7, f_8)$
- Unknown (4 variables):
  - → ρ_w
  - → $f_q = (f_2, f_5, f_6)$
- 3 Equations (2 linearly independent):
  - → $\sum f_q = \rho_w$
  - → $\sum \mathbf{c}_q f_q = \rho_w \mathbf{u}_w$

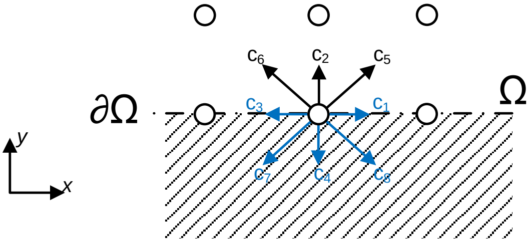
Boundary conditions in LBM



- Symmetry of $f_q^{(\mathrm{neq})}$ (3 equations):
  - → Bounce-back of non-equilibrium populations
- Introduce extra variable (problem over-specified):
  - → Transverse momentum correction N_{xy}
- Problem is well specified:
  - → 6 eqs. and 6 unknowns

Boundary conditions in LBM

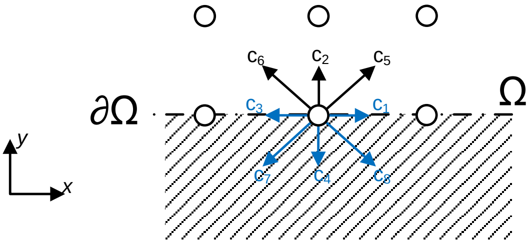
1) Computing ρ_w...



- 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...



- Relate the two velocity moments:

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

- Solution:

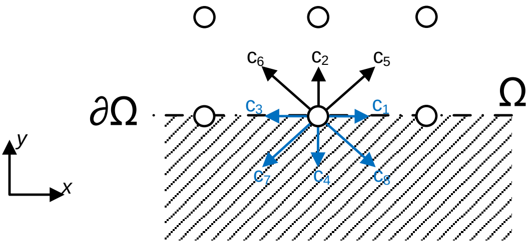
$$\rho_w = \rho_w u_{y_w} + \rho_0 + 2\rho_-$$

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

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

Boundary conditions in LBM

2) Computing $\{f_2, f_5, f_6\}$**...**



- 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 $\{f_2, f_5, f_6\}$...

Solution for the unknown incoming populations:

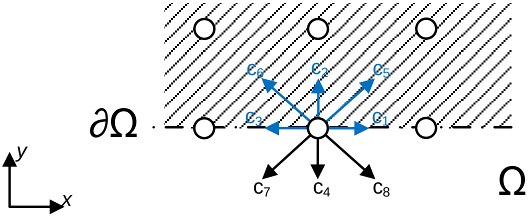
$$f_2 = f_4 + \frac{2}{3}\rho_w\, u_{y_w}$$

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

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

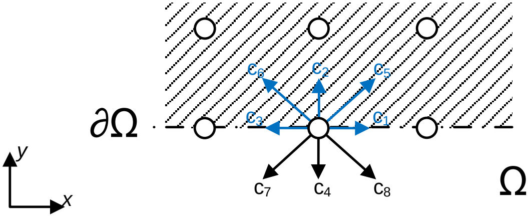
Question:

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:

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

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

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

- Solution:

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

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

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

Question: Boundary conditions in LBM

2) Computing $\{f_4, f_7, f_8\}$**...**

Solution for the unknown incoming populations:

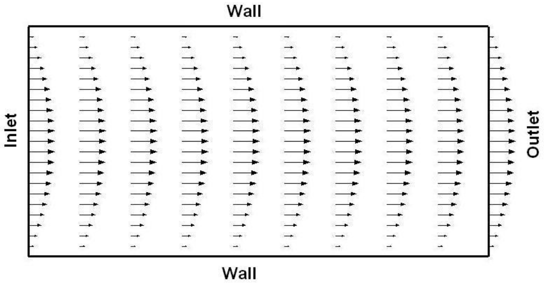
$$f_4 = f_2 - \frac{2}{3}\rho_w\, u_{y_w}$$

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

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

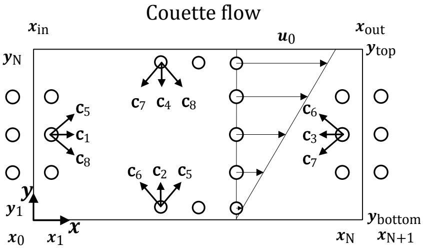
Numerical Lab

Testing the LBM for different BC schemes

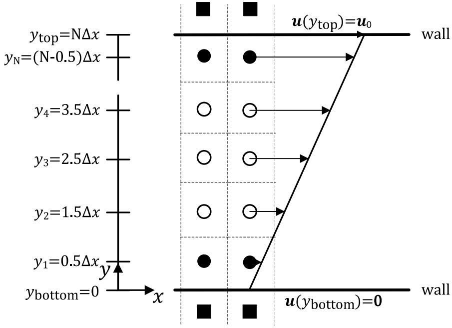


Exercise I:

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 $j = 1, 2, \ldots, N_y$.

Input parameters

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

  and

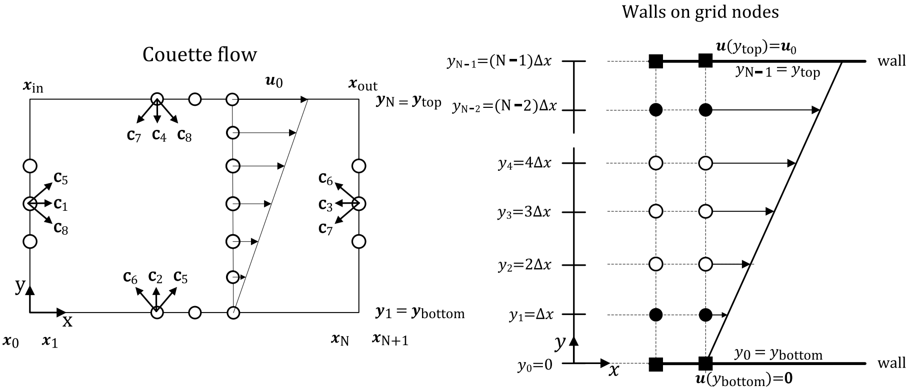
- $\mathbf{U_{max}}$ → Maximum velocity (proportional to Mach number)
- or τ → Relaxation time (LBM parameter)

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 $Re = 0.1$

Exercise II:

Couette flow in channel with NEBB boundaries



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

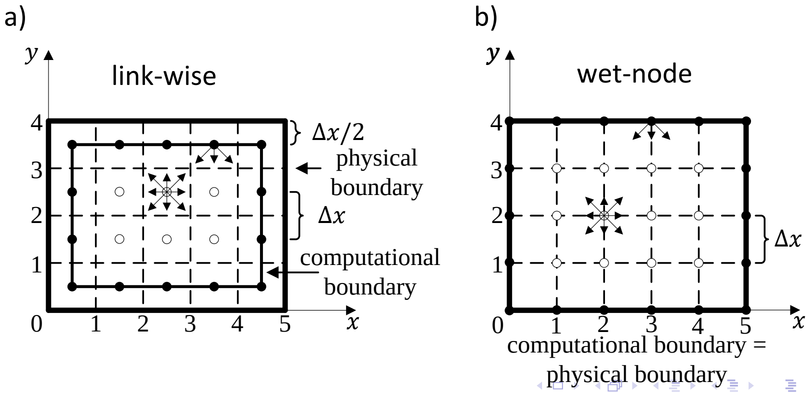
Couette flow in channel with NEBB boundaries

- **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 $Re = 0.1$

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

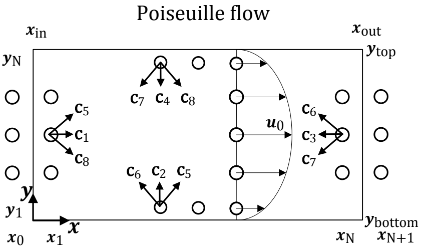
Question: Where are grid nodes located in computational cells?

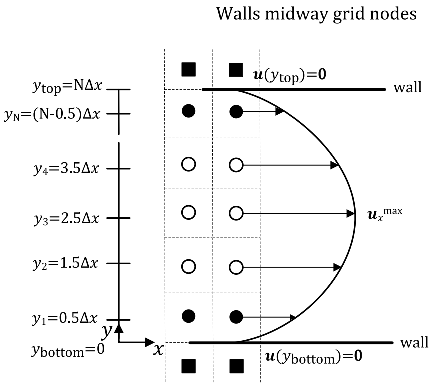
a) Grid nodes are cell centred **b)** Grid nodes are vertex centred



Exercise III:

Poiseuille flow in channel with BB 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: $\mathrm{Re} = \frac{u_0\,L_y}{\nu}$ where $L_y = N_y\,\Delta x$.
- **Bounce-back walls:** $y_j = -\frac{\Delta x}{2} + j\,\Delta x$ where $j = 1, 2, \ldots, N_y$.

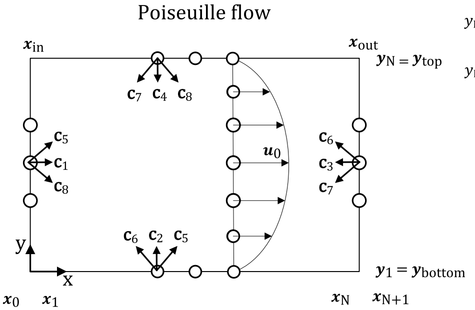
Poiseuille flow in channel with BB boundaries

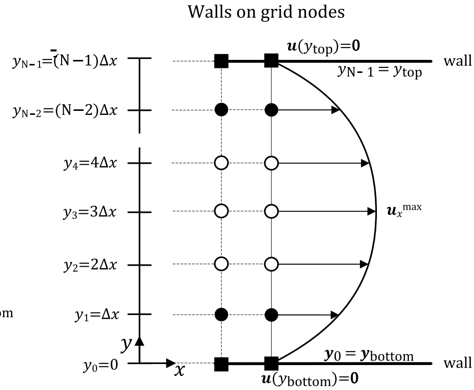
- **Question 1:** Fix $Re = 10$ and $\tau = 0.9$
  - **Question 1.1** For $N_y = 16$, what is U_{max} and $\|L_2\|$ error norm?
  - **Question 1.2** For $N_y = 32$, what is U_{max} and $\|L_2\|$ error norm?
  - **Question 1.3** Estimate the convergence rate

    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: $\text{Re} = \frac{u_0\,L_y}{\nu}$ where $L_y = N_y\,\Delta x$.
- **Bounce-back walls:** $y_j = (j-1)\,\Delta x$ where $j = 1, 2, \ldots, N_y$.

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