Lattice Boltzmann Method: Basic theory and applications

Overview

- ➢Introduction: What is the LBM?
- ➢Theory:
  - Important scales
  - Distribution Functions, The Boltzmann Equation & Collision Operators
  - LBM vs Conventional Methods (vs Particle Based Methods)
  - Discretisation & Velocity Sets
  - Collision & Streaming
- ➢Implementation:
  - Initialisation
  - Boundary Conditions
  - Timestep Algorithm
- ➢Applications
  - Why LBM?
  - Why not LBM?
  - LBM vs FVM

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The Lattice Boltzmann Method

- First emerged in the 1980s as an alternative to conventional (NS) methods for CFD.
- Highly parallelable leading to revived interest recently due to advances in GPU performance.
- Mesoscopic treatment of collision allows for modelling of complex fluid-structure interactions which NS struggles with (porous materials, biomedical applications, multiphase flows, surface / capillary flows)

Who was Boltzmann?

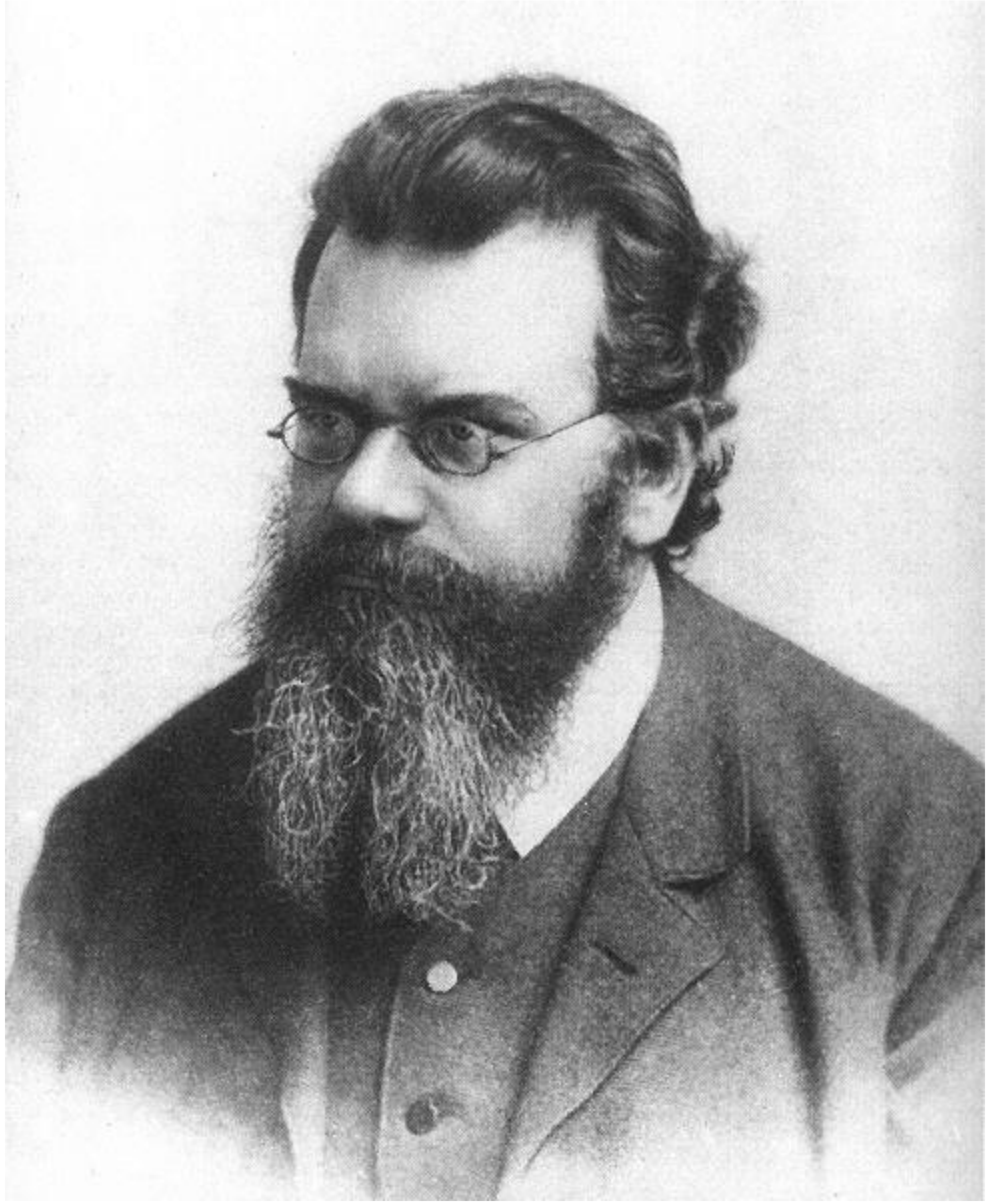
- Ludwig Eduard Boltzmann (1844 – 1906) was an Austrian physicist known for his contribution to **statistical mechanics.**
- Notable work:
    - Second law of thermodynamics and statistical order:

$$\boldsymbol{S = k_b \ln W}$$

    - Gas dynamics and continuum mechanics:

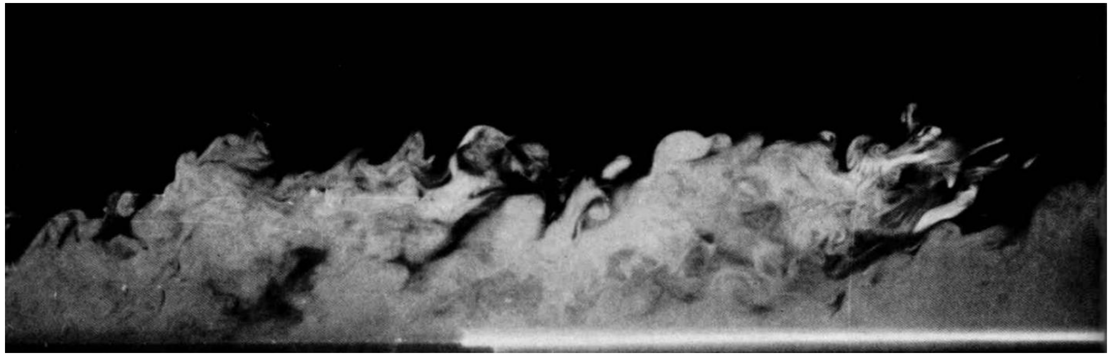
$$\boldsymbol{\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{F}{m}\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t}_{Collision}}$$

    - Atomic Theory and Quantum Mechanics



Fluid Mechanics: Boltzmann Vs Navier and Stokes

- NS treat fluids as a continuum describing **macroscopic** quantities such as viscosity and pressure.



- At microscopic these quantities don’t exist

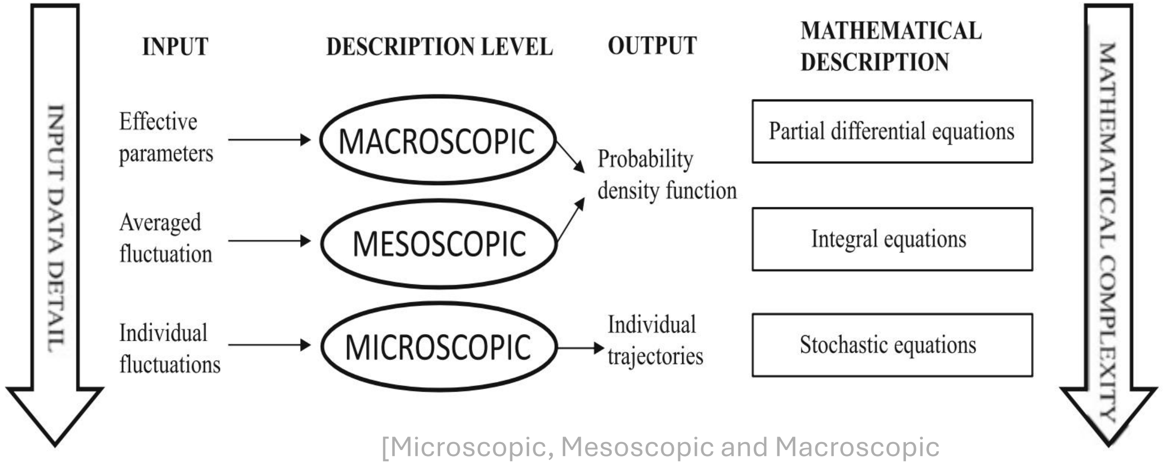
- Boltzmann models the intermediate scale - mesoscopic

Important Scales

- Microscopic:
  - Interactions between individual particles/molecules.
  - Newtonian dynamics describing deterministic collisions.
  - **Discontinuous**

- Mesoscopic:
  - Ensembles of particles.
  - **Kinetic theory** describing the evolution of statistical quantities.
  - **Statistical**

- Macroscopic:
  - A continuous medium.
  - Macroscopic quantities: **viscosity, pressure, density**
  - Described by NSE using smooth variables.
  - **Continuous**



[Microscopic, Mesoscopic and Macroscopic Descriptions of Dispersal, Mendez, 2023.]

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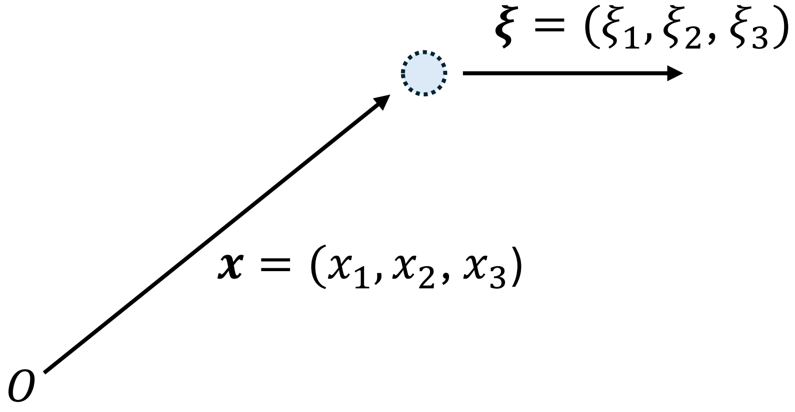
Statistical Representation of Particles

- The (particle) distribution function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ **is the density of particles moving with microscopic particle velocity $\boldsymbol{\xi}$**, at position $\boldsymbol{x}$ in space, at time t.
- It is a *generalisation* of the macroscopic density.



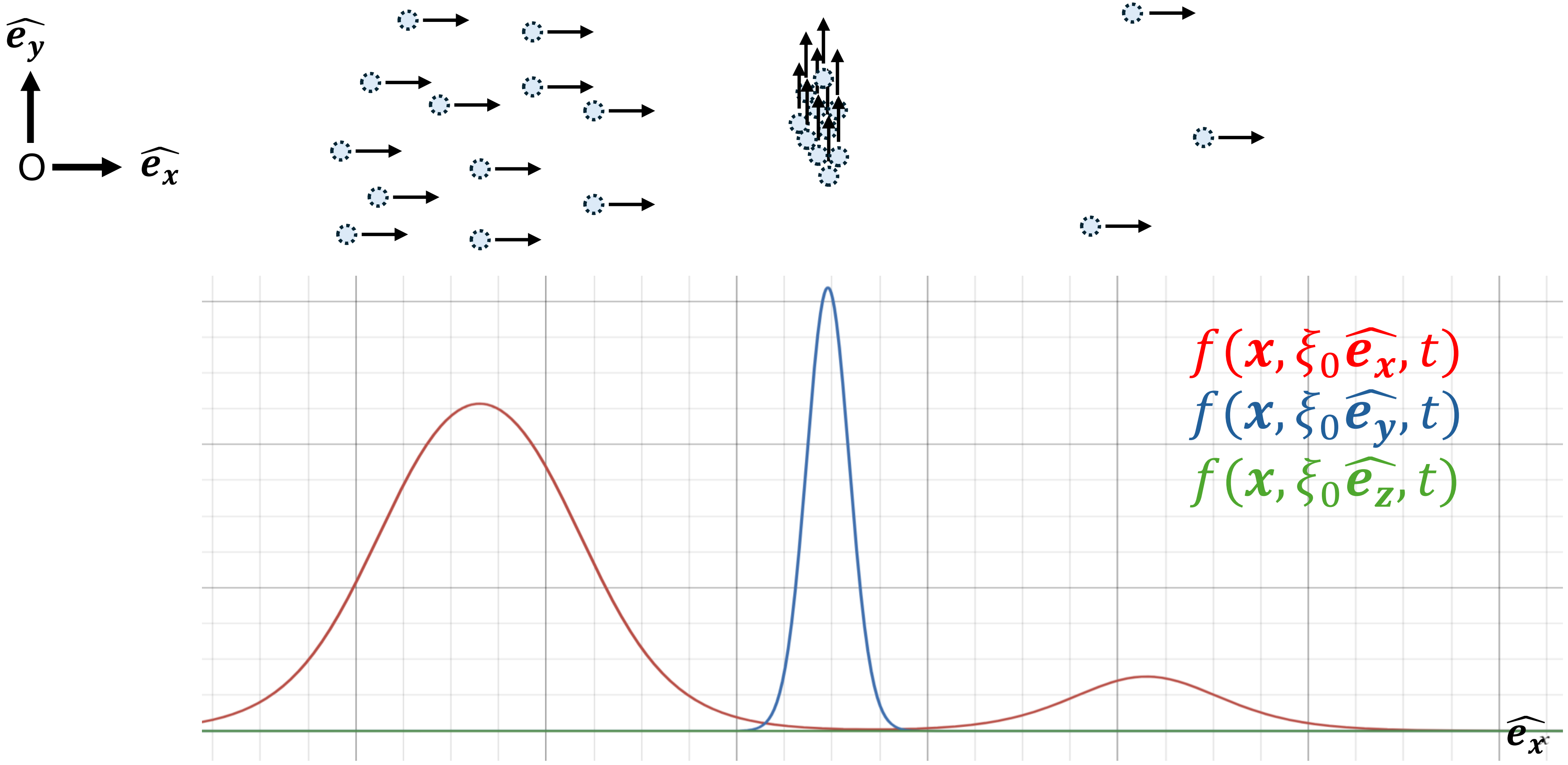
i.e. at $(\boldsymbol{x}, t)$ there is a density of particles moving with velocity $\boldsymbol{\xi}$.

Note: $\boldsymbol{\xi} \in \mathbb{R}^3$

Distribution Function: An Example

- What would a plot of f look like?

Assume all $|\boldsymbol{\xi}| = \xi_0$

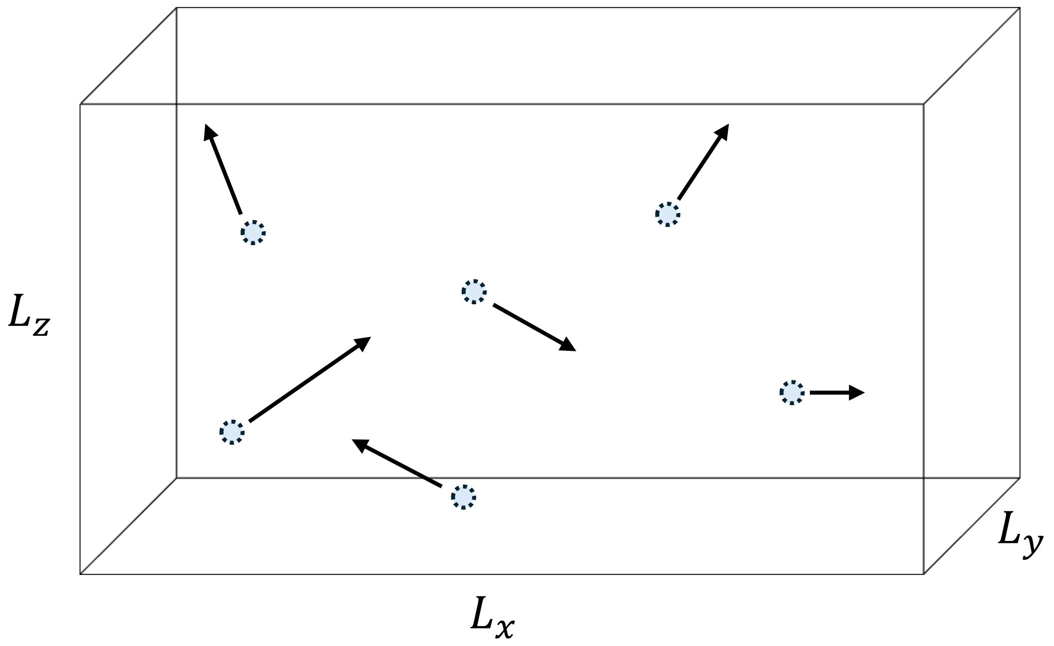


Distribution Function: Another Example

- Consider a box given by with dimensions L_x, L_y, L_z.
- What is the density of *right-moving* $(\xi_x > 0)$ particles within the box?
- Ans: $$\iiint_V \iiint_{\xi_x>0} f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3 dx^3$$

Volume integral over box

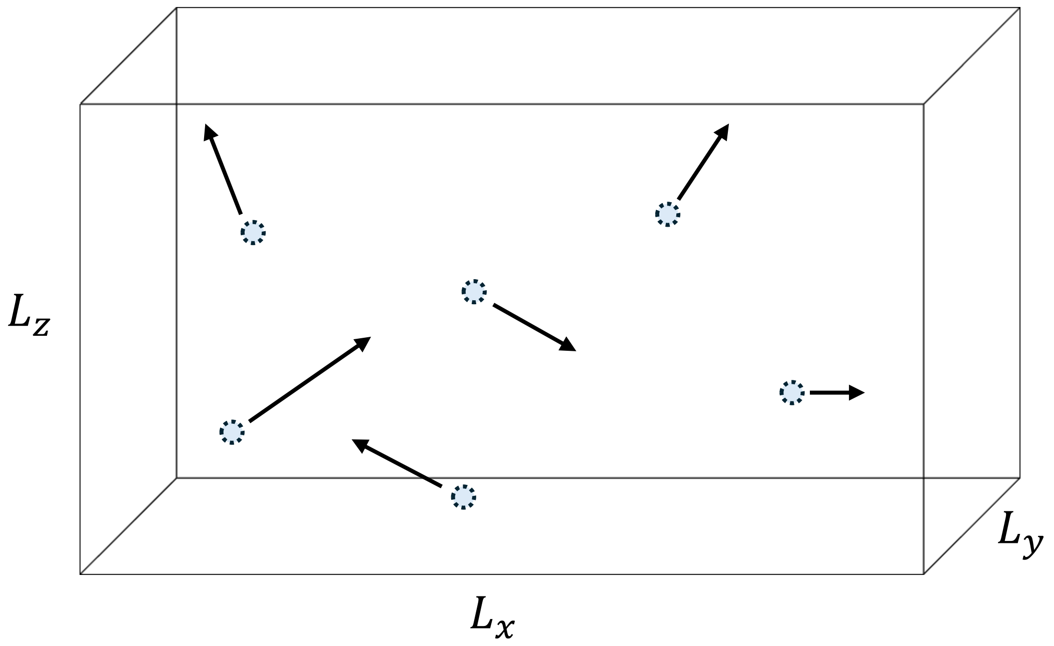
Integrating over all possible velocities with $\xi_x > 0$



Moments of The Distribution Function

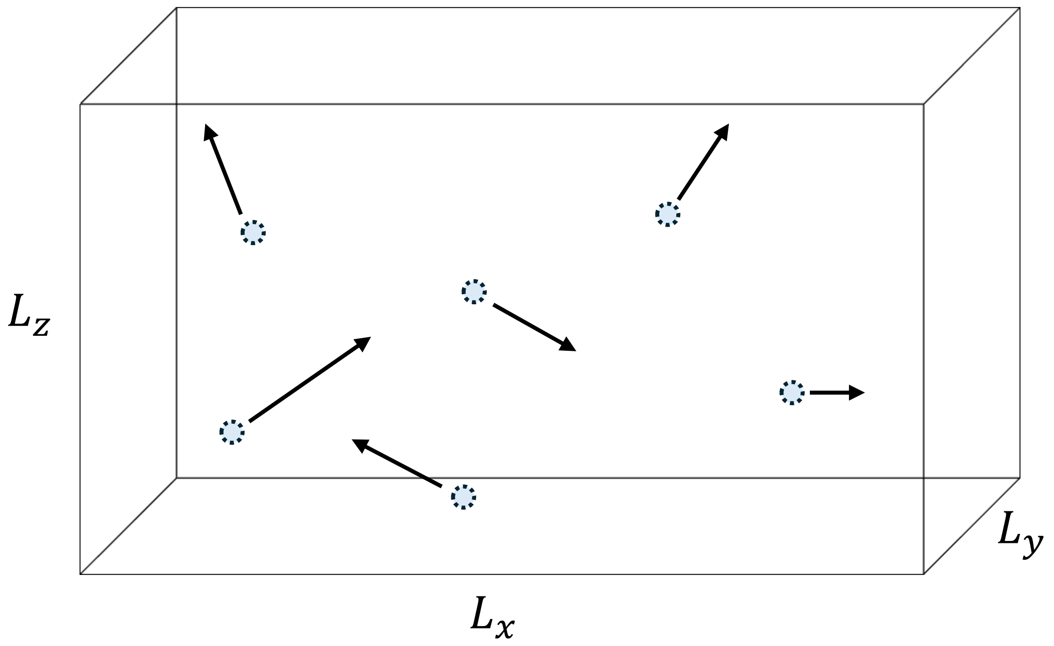
- The distribution function is the statistical representation of the microscopic behaviour?

- How does it relate to the macroscopic behaviour?



Moments of The Distribution Function

- How do we find the density at the position $(\boldsymbol{x}, t)$?
- Integrate over all possible velocities to return to a *conventional* density function.



$$\rho(\boldsymbol{x}, t) = \iiint\limits_{\boldsymbol{\xi} \in \mathbb{R}^3} f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3$$

Integrating over all possible velocities

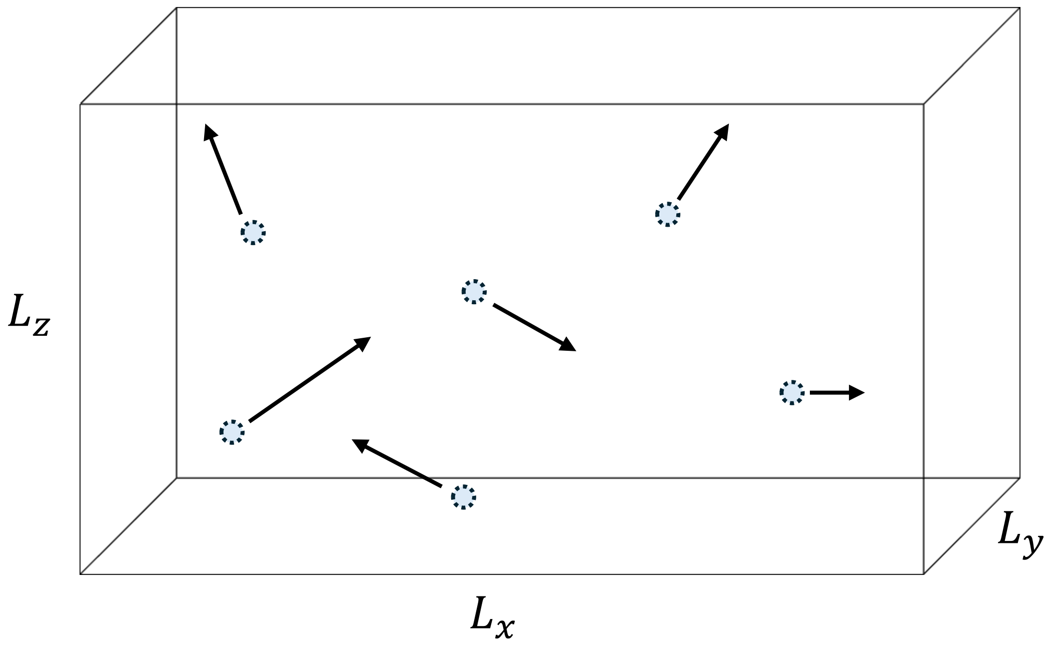
The zeroth moment of the distribution function is the density

Moments of The Distribution Function

- How do we find the velocity at the position $(\boldsymbol{x}, t)$?
- Each particle contributes $\boldsymbol{\xi} f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ to the momentum density.

$$\boldsymbol{u}(\boldsymbol{x}, t)\rho(\boldsymbol{x}, t) = \iiint_{\boldsymbol{\xi} \in \mathbb{R}^3} \boldsymbol{\xi} f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3$$

$$\boldsymbol{u}(\boldsymbol{x}, t) = \frac{\iiint_{\boldsymbol{\xi} \in \mathbb{R}^3} \boldsymbol{\xi} f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3}{\iiint_{\boldsymbol{\xi} \in \mathbb{R}^3} f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3}$$

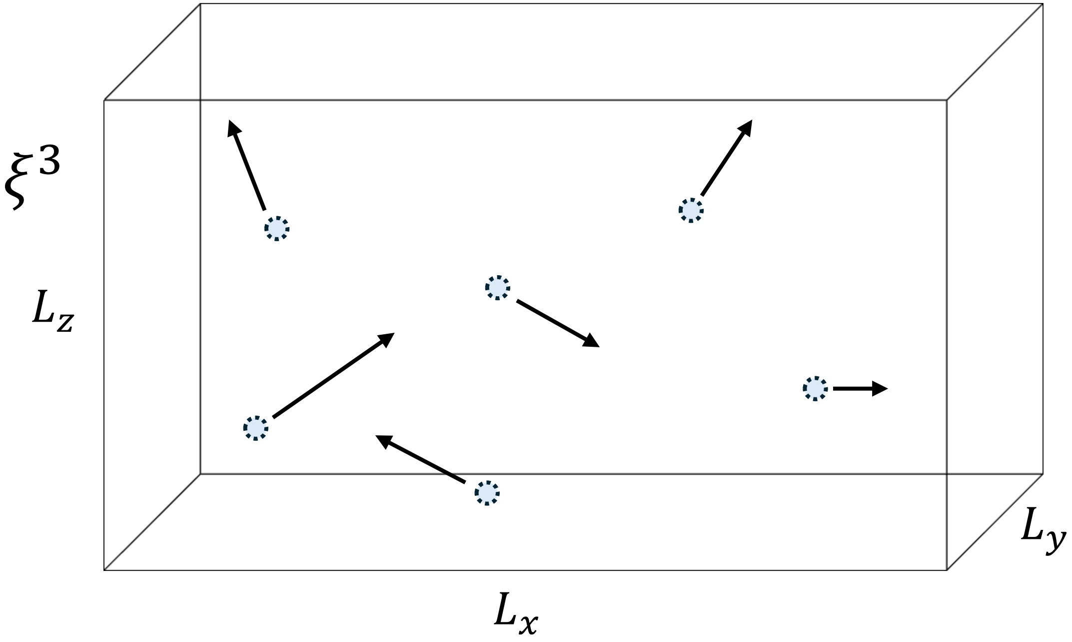


The first moment of the distribution function is the momentum

Moments of The Distribution Function

- How do we find the **total energy** at the position $(\boldsymbol{x}, t)$?

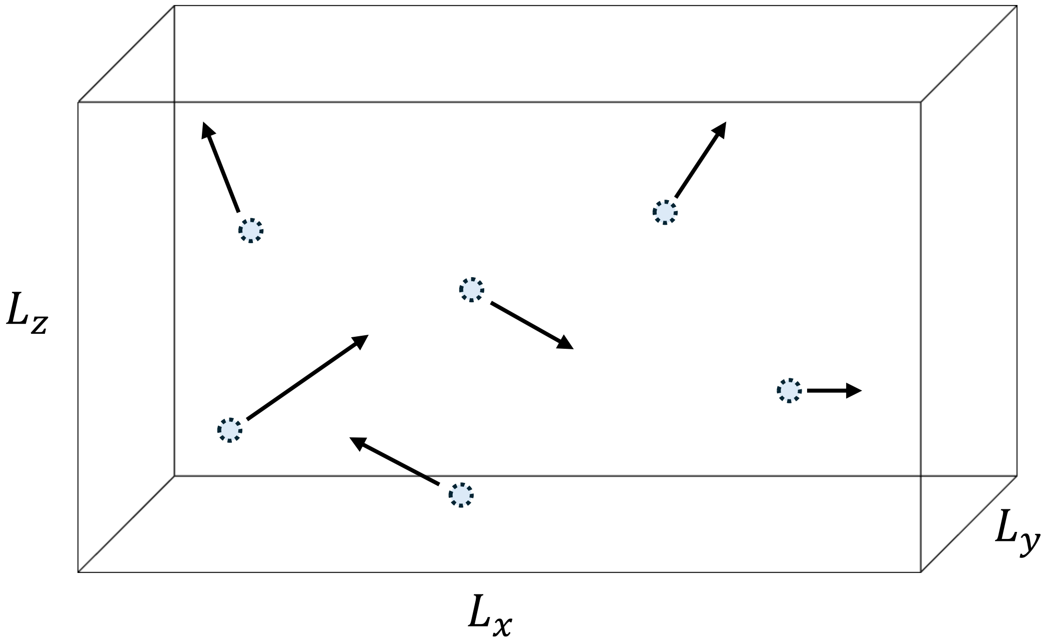
$$E(\boldsymbol{x}, t) = |\boldsymbol{u}(\boldsymbol{x}, t)|^2 \rho(\boldsymbol{x}, t) = \iiint_{\boldsymbol{\xi} \in \mathbb{R}^3} |\boldsymbol{\xi}|^2 f(\boldsymbol{x}, \boldsymbol{\xi}, t) d\xi^3$$



- $E(\boldsymbol{x}, t)$ is **NOT** the kinetic energy in a macroscopic sense.
- It is the microscopic kinetic energy.
- Thermal energy + bulk flow kinetic energy (macroscopic KE)

The Equilibrium Density Function

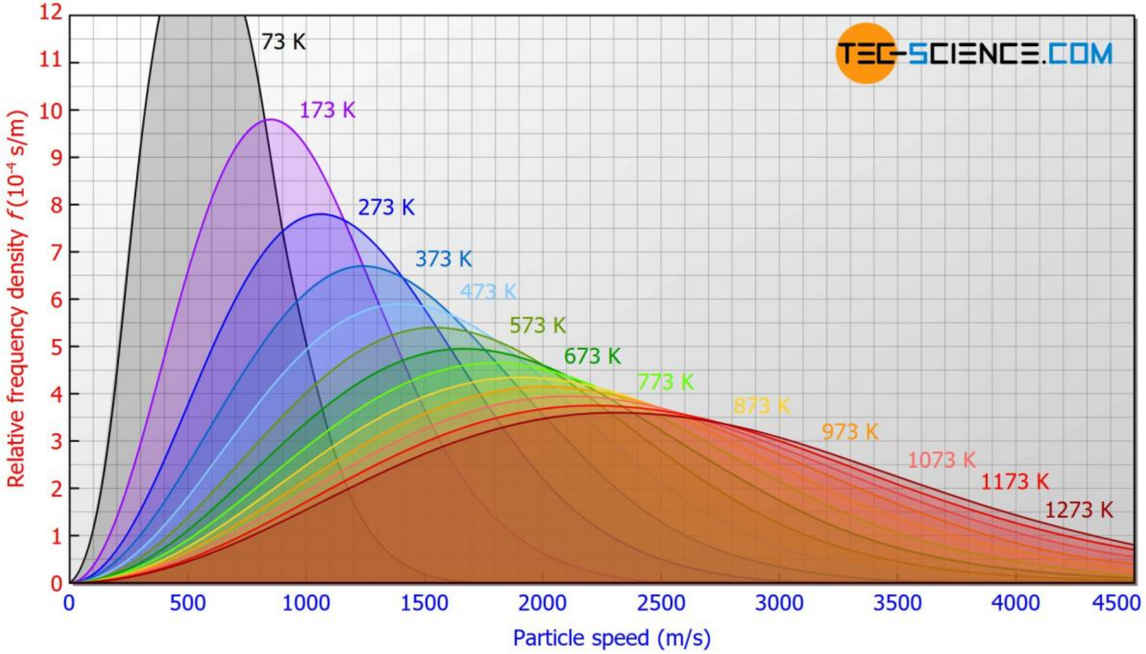
- Suppose we leave our box for a long time.
- It will tend to some equilibrium state.
- This can be represented by the equilibrium density function.
- We assume:
  - It is isotropic in $\boldsymbol{\xi}$-space around some velocity $\boldsymbol{u}$
  - It is separable in the components of the reference velocity.



The Equilibrium Density Function

- $f^{eq}(|\boldsymbol{v}|^2) = f^{eq}(v_x^2 + v_y^2 + v_z^2) = f_{1D}^{eq}(v_x^2) f_{1D}^{eq}(v_y^2)\, f_{1D}^{eq}(v_z^2)$
- Holding magnitude of $|\boldsymbol{v}|^2$ = const, then
- $\ln\left(f_{1D}^{eq}(v_x^2)\right) + \ln\left(f_{1D}^{eq}(v_y^2)\right) + \ln\left(f_{1D}^{eq}(v_z^2)\right) = \text{const}$
- And thus $\ln\left(f_{1D}^{eq}(v_i^2)\right) = a + bv_i^2$ for constants a, b
- So finally $f^{eq}(|\boldsymbol{v}|^2)$ must take the form
- $f^{eq}(|\boldsymbol{v}|^2) = e^{3a} e^{b|\boldsymbol{v}|^2}$.
- Using the conservation of mass and momentum we can find the constants.

- $\Rightarrow\ f^{eq}(\boldsymbol{x}, |\boldsymbol{v}|, t) = \rho\left(\frac{1}{2\pi RT}\right) e^{-\frac{|v|^2}{2RT}}$
- The Maxwell-Boltzmann Distribution.



[Tec-Science.com]

The Boltzmann Equation

- We know that with no external changes as $t \to \infty$, $f \to f^{eq}$.
- But how does it do this?
- We want to find understand the evolution of f.

The Boltzmann Equation

- The total derivative of $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is:

$$\frac{df}{dt} = \frac{\partial f}{\partial t}\underbrace{\frac{dt}{dt}}_{=1} + \frac{\partial f}{\partial x_\beta}\underbrace{\frac{dx_\beta}{dt}}_{=\xi_\beta} + \frac{\partial f}{\partial \xi_\beta}\underbrace{\frac{d\xi_\beta}{dt}}_{=\frac{F_\beta}{\rho}}$$

By Newtons Second
Law for some body
force $\boldsymbol{F}$

The Boltzmann Equation

- This must be equal to some source term, $\Omega(f)$:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\rho}\frac{\partial f}{\partial \xi_\beta} = \Omega(f)$$

Distribution function is advected with the particle velocity ξ_β

Effects of forcing

Source term effecting mesoscopic evolution due to microscopic collisions

The Collision Operator

- The collision operator must:

1. Conserve mass $$\int \Omega(f) d^3\xi = 0$$
2. Conserve Momentum $$\int \boldsymbol{\xi}\Omega(f) d^3\xi = \mathbf{0}$$
3. Conserve total energy* $$\int |\boldsymbol{\xi}|^2\Omega(f) d^3\xi = 0$$

* Assuming monatomic particles

The BGK Collision Operator

- Named after Bhatnagar, Gross and Krook
- Links f to f^{eq} by some relaxation time τ.

$$\Omega(f) = -\frac{1}{\tau}\left(f - f^{eq}\right)$$

Small τ ⇒ fast convergence to f^{eq}
Large τ ⇒ slow convergence to f^{eq}

Viscosity!*

This is just one choice of $\Omega(f)$!

* And heat diffusivity

Stability of The BGK Collision Operator

$$\Omega(f) = -\frac{1}{\tau}\,(f\ - f^{eq})$$

- If $\frac{\tau}{\Delta t} = 1, f$ decays directly to f^{eq}
- If $\frac{\tau}{\Delta t} > 1, f$ decays exponentially towards f^{eq}
- If $\frac{1}{2} < \frac{\tau}{\Delta t} < 1, f$ converges towards f^{eq} via decaying oscillations
- If $\frac{1}{2} \leq \frac{\tau}{\Delta t}, f$ diverges from f^{eq}

* And heat diffusivity

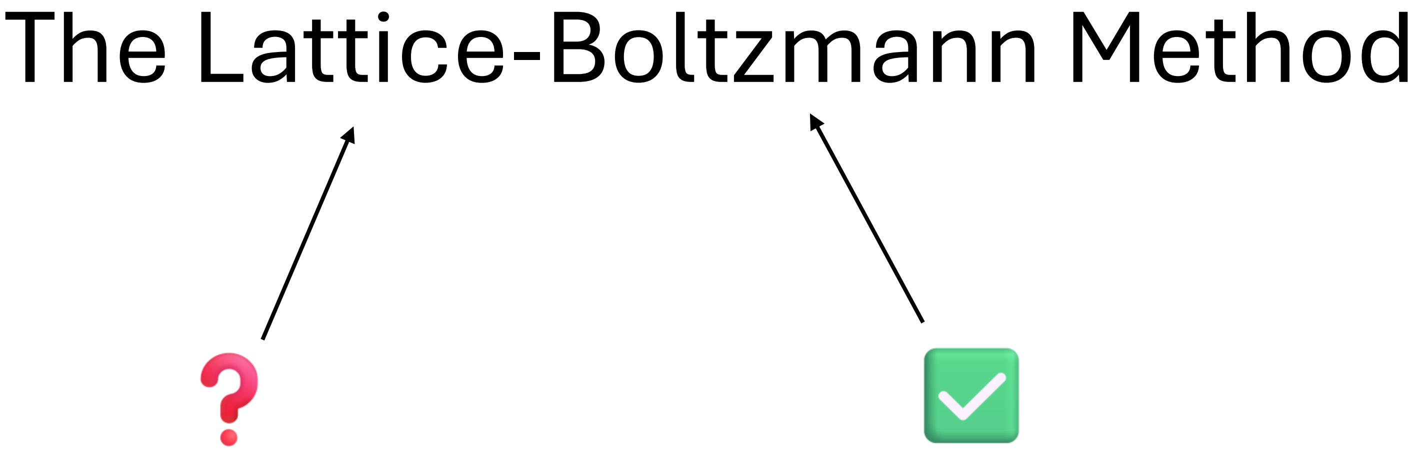
A Quick Summary

1. f represents a velocity density
2. Macroscopic quantities are found from the moments of f
3. f evolves according to

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\rho} \frac{\partial f}{\partial \xi_\beta} = -\frac{1}{\tau}\left(f - f^{eq}\right)$$

4. We can tune τ to fluid properties

The LBM



The Lattice-Boltzmann Method

❓ ✅

Motivation For A Lattice

For some f, calculate ρ.

Easy, right?...

$$\rho(\boldsymbol{x}, t) = \int f(\boldsymbol{x}, \boldsymbol{\xi}, t) d^3\xi$$

What does this really mean?

$$\rho(\boldsymbol{x}, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\boldsymbol{x}, \xi_1, \xi_2, \xi_3 t) d\xi_1 d\xi_2 d\xi_3 \Rightarrow$$ 😳 😔 😭

Motivation For A Lattice

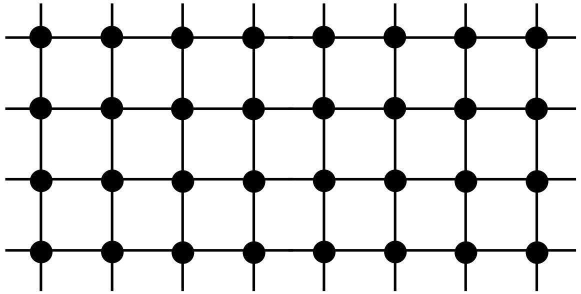
What if we choose some finite set $\boldsymbol{\xi} \in \{\boldsymbol{c}_i\}$?

$$\rho(\boldsymbol{x}, t) = \sum_i f(\boldsymbol{x}, \boldsymbol{\xi}_i, t) \text{ ✅}$$

$\{\boldsymbol{c}_i\}$ is known as a *velocity set*

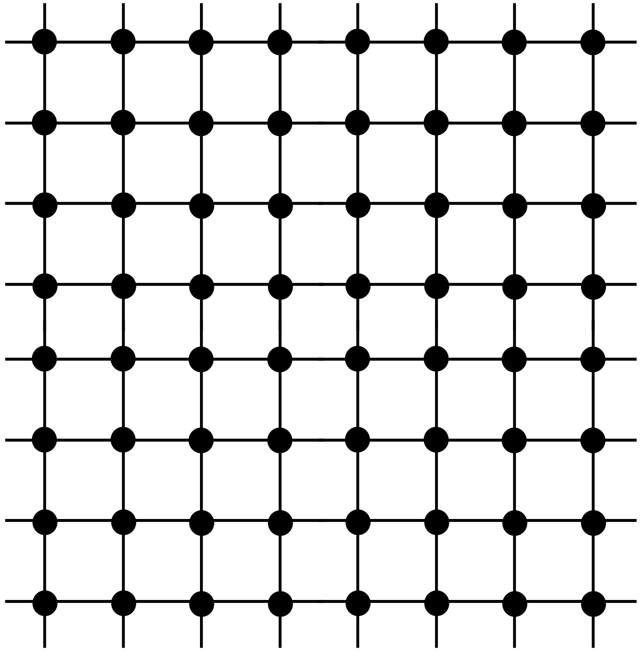
Imagine we have $\{\boldsymbol{\xi}_i\} = \{(1,0),\ (0,1),\ (0,-1), (-1,0)\ , (0,0)\}$

Then every point on a square lattice can jump to its neighbour



Motivation For A Lattice

- By using a lattice, we can discretise our domain into **connected** points.
- This ensures we don't *lose* particles as they traverse the domain



Continuous	**Discrete**
$\boldsymbol{\xi}$	$\{\boldsymbol{c}_i\}$
t	Δt
$\boldsymbol{x}$	$\sum_i a_i \boldsymbol{c}_{\boldsymbol{i}} \, \Delta t$

Velocity Weighting

- For each $\boldsymbol{c}_i$, define some weight w_i

- Weighting ensures conservation laws…

$$\sum_i f_i = \rho$$

$$\sum_i \boldsymbol{c_i} f_i = \rho \boldsymbol{u}$$

where $f_i = w_i f(\boldsymbol{x}, \boldsymbol{c_i}, t)$

Finding Suitable Weights

- Finding a suitable weighting requires more work
- For a NS solver, weights must obey:

$$
\begin{aligned}
\sum_i w_i &= 1, \\
\sum_i w_i c_{i\alpha} &= 0, \\
\sum_i w_i c_{i\alpha} c_{i\beta} &= c_s^2 \delta_{\alpha\beta}, \\
\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} &= 0, \\
\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\mu} &= c_s^4 (\delta_{\alpha\beta}\delta_{\gamma\mu} + \delta_{\alpha\gamma}\delta_{\beta\mu} + \delta_{\alpha\mu}\delta_{\beta\gamma}), \\
\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\mu} c_{i\nu} &= 0.
\end{aligned}
$$

As a result of quadrature rules

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) \approx \omega(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \cdot \boldsymbol{H}^{(n)}(\boldsymbol{\xi}).$$

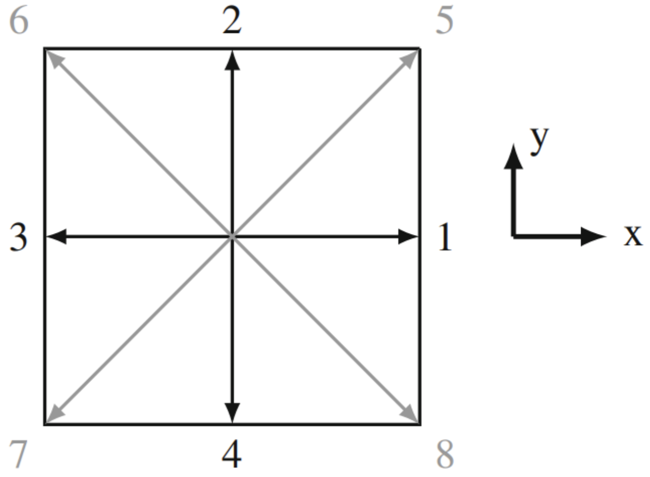
Velocity Naming Scheme

DdQq

dimensions

velocities

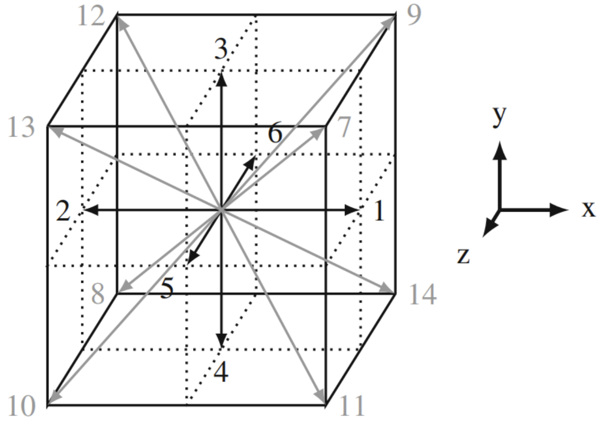
D1Q3



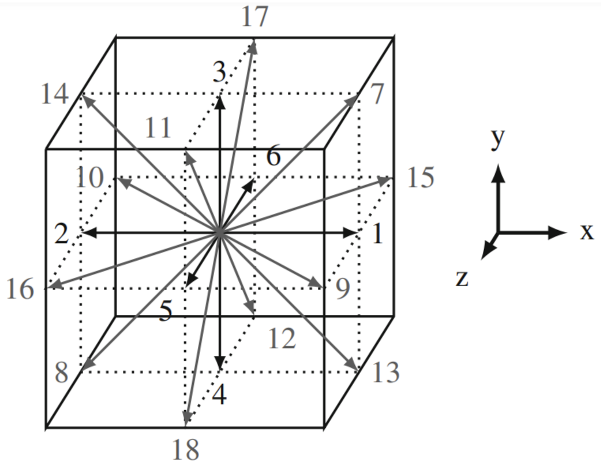
D2Q9

[The Lattice Boltzmann Method Principles and Practice, Kruger et al, 2016]

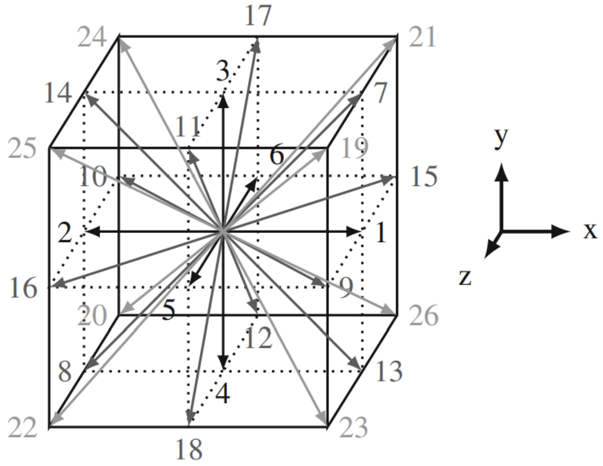
Velocity Naming Scheme



D3Q15



D3Q19



D3Q27

[The Lattice Boltzmann Method Principles and Practice, Kruger et al, 2016]

Lattice Boltzmann Equation

Assuming no body forces ($F_\beta = 0$)

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\rho}\frac{\partial f}{\partial \xi_\beta} = \Omega(f)$$

Using 1st order discretisation, we get

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t) + \Delta t \, \Omega_i(\boldsymbol{x}, t)$$

The *“Lattice Boltzmann Equation”*.

With a redefinition of Ω_i, this is equivalent to a 2nd time discretisation.

An interpretation

The LBE:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t) + \Delta t \, \Omega_i(\boldsymbol{x}, t)$$

Imagine instead, $\boldsymbol{x}_i' = \boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}$ and $\mathrm{t}' = \mathrm{t} + \Delta t$

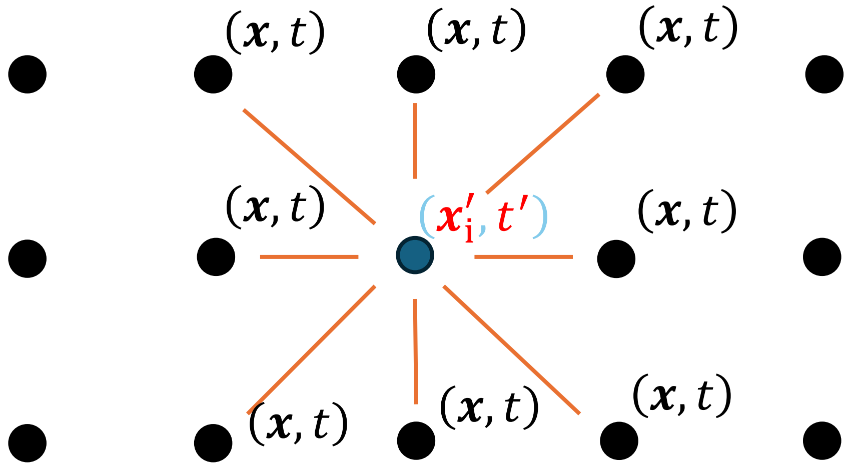
$\boldsymbol{x}_i'$ represents the neighbours of $\boldsymbol{x}$

They share information at t'

An interpretation

The LBE:

$$f_i(\boldsymbol{x}'_{\mathrm{i}}, t') = f_i(\boldsymbol{x}, t) + \Delta t\, \Omega_i(\boldsymbol{x}, t)$$



An interpretation

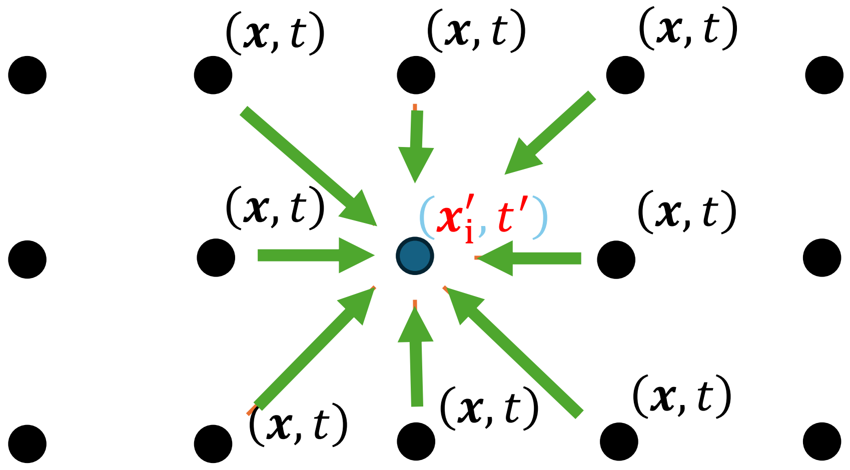
The LBE:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t) + \Delta t \; \Omega_i(\boldsymbol{x}, t)$$

This is the streaming term:

From $\boldsymbol{x}$, the distribution function f_i is "*streamed*" to its i^{th} neighbour

The particles move from one neighbour to the next



An interpretation

The LBE:

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An interpretation

The LBE:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t) + \Delta t \ \Omega_i(\boldsymbol{x}, t)$$

New Distribution = Streamed Distribution + Collisions

Discrete Equilibrium Functions

After some manipulation…

$$f_i^{eq} = w_i\rho\left(1 + \frac{c_{i\alpha}u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})}{2c_s^2}\right)$$

Where c_s is the speed of sound and be calculated with

$$c_s^2 = w_i(\boldsymbol{c} \cdot \boldsymbol{c})_i$$

For all velocity sets shown $c_s^2 = \frac{1}{\sqrt{3}}$

(Another) Quick Summary

- We have discretised the Boltzmann Equation into the LBE

Streaming Collision

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t) + \Delta t\ \Omega_i(\boldsymbol{x}, t)$$

$$f_i^{eq} = w_i \rho \left(1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta})}{2 c_s^2} \right)$$

- Using a velocity set $\{c_i\}$ forming a lattice of points $\{\boldsymbol{x}_i\}$

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Initialisation

- We have some field $\boldsymbol{u}_0$ at time $t = 0$

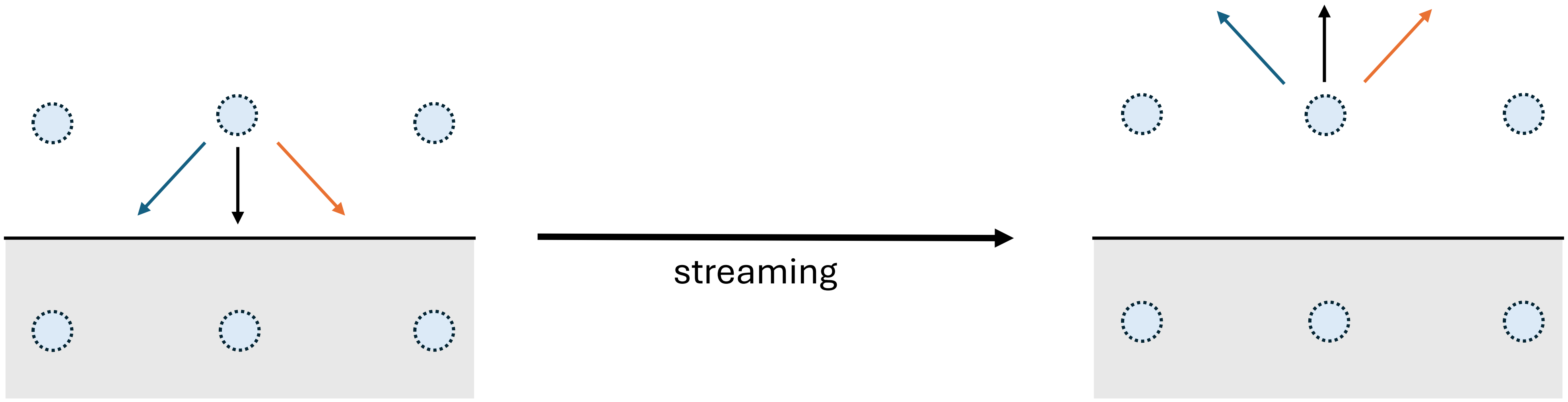
- The simplest way to initialise is to assume equilibrium…

$$f(\boldsymbol{\xi}, \boldsymbol{u}, t) = f^{eq}(\boldsymbol{\xi}, \boldsymbol{u}_0, 0)$$

This is not always appropriate especially with high velocity gradients

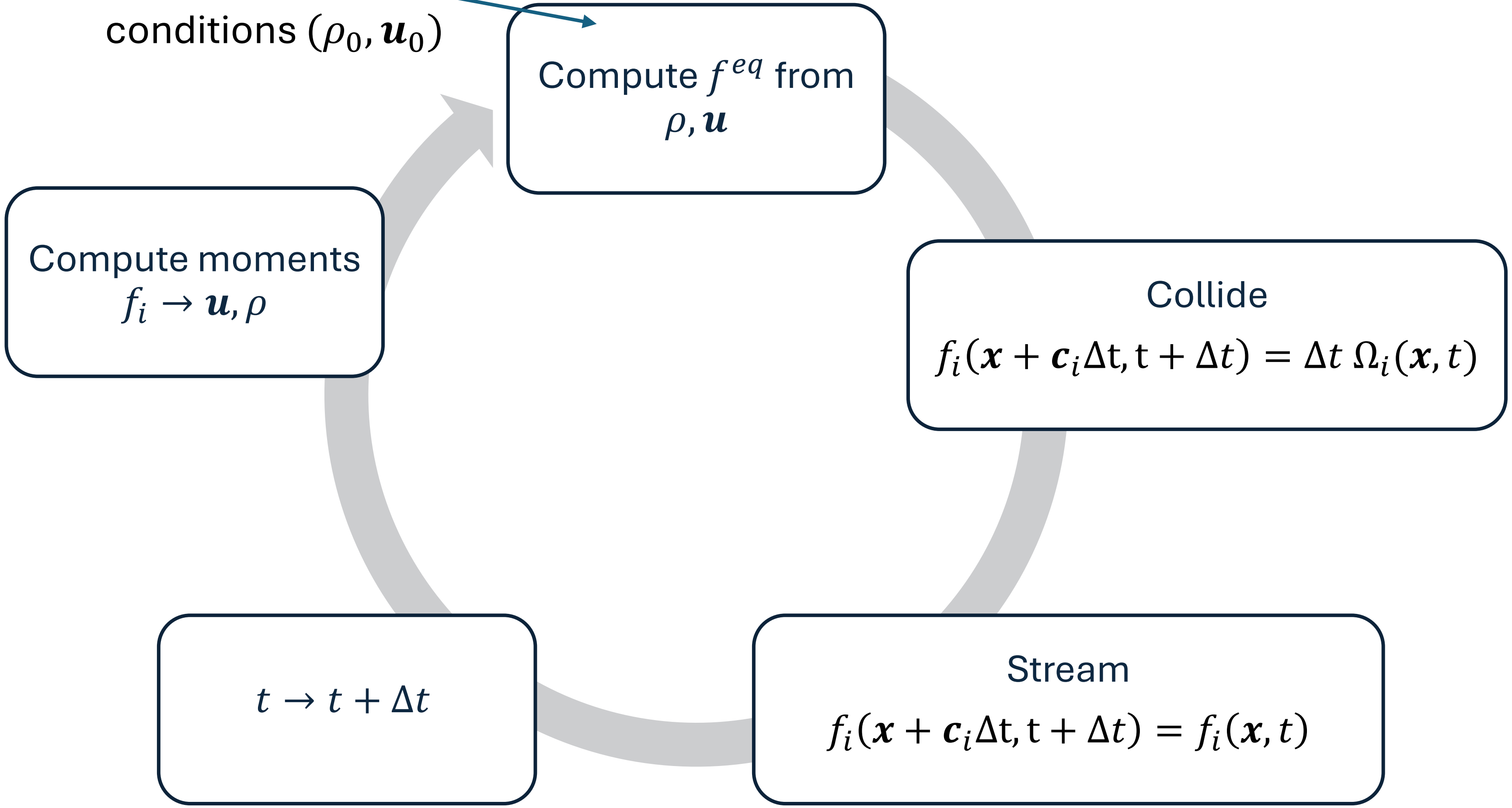
Boundary Conditions: No Slip

- We want to impose $\boldsymbol{u} = \mathbf{0}$ on walls
- The simplest option is the *“Bounce-Back Condition”*



- The distribution function is reflected

Timestep Algorithm



Provide initial conditions $(\rho_0, \boldsymbol{u}_0)$

Compute f^{eq} from $\rho, \boldsymbol{u}$

Collide

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = \Delta t\ \Omega_i(\boldsymbol{x}, t)$$

Stream

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta \mathrm{t}, \mathrm{t} + \Delta t) = f_i(\boldsymbol{x}, t)$$

$t \rightarrow t + \Delta t$

Compute moments $f_i \rightarrow \boldsymbol{u}, \rho$

An Example

…

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Advantages of LBM

- Nonlinearity is contained entirely within the collision operator $\Omega(f)$
- Meaning nonlinearity is **local**
- Grid points are independent (after streaming)
- Operations have excellent uniformity
- Decomposition of a regular lattice is easy
- Data handover is minimal
- Direct modelling of microscopic collisions allows for better modelling

Disadvantages of LBM

- The domain is limited to regular lattices
- It is only weakly incompressible
- It is not suitable for steady-state simulations
- It is extremely memory intensive…

Memory usage of LBM

- Consider a 100x100x100 grid of D3Q27 points
- Each point must store

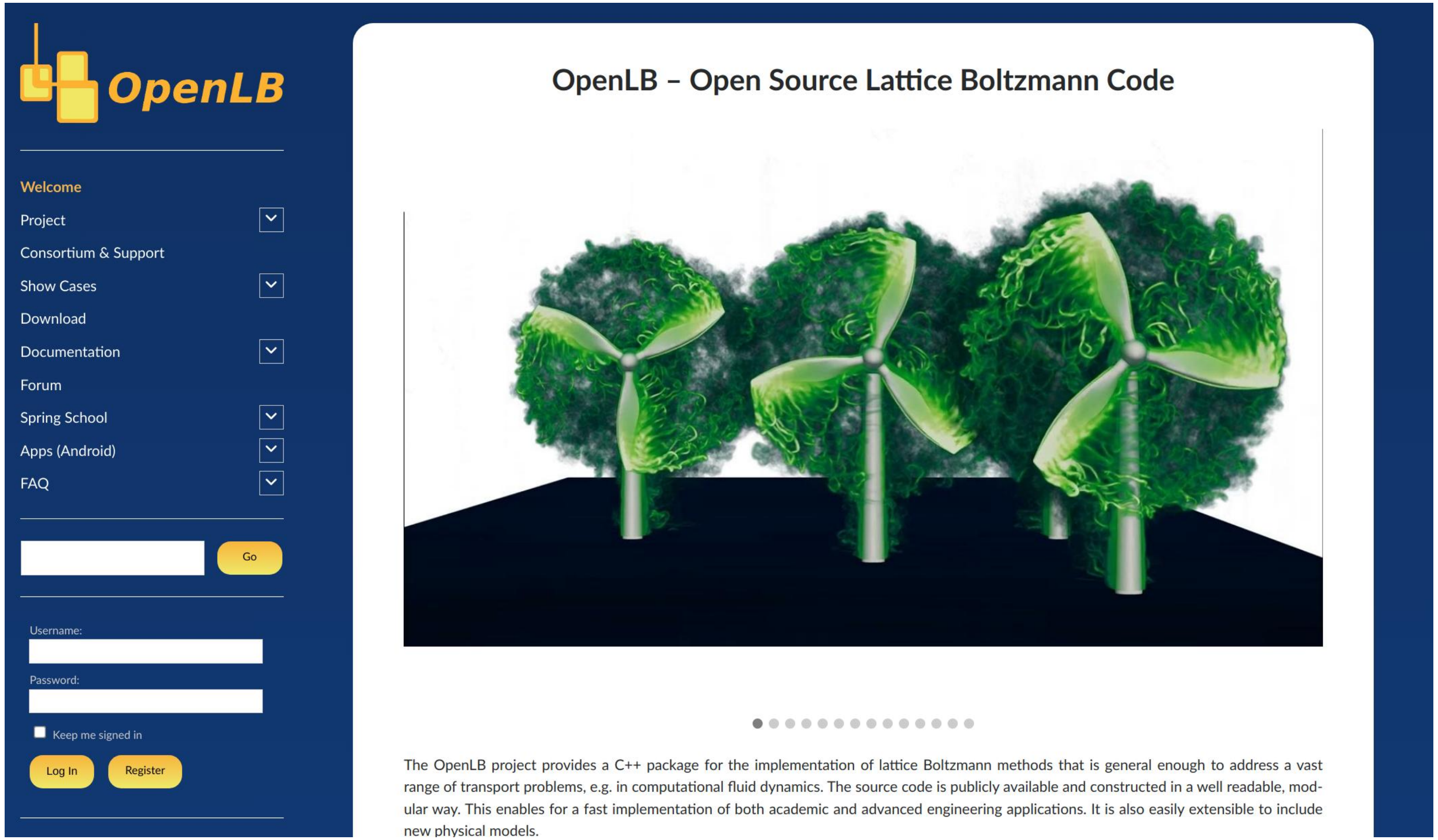
$$(u_1, u_2, u_3)$$
$$\rho$$
$$f_1, f_2, f_3, f_4, f_5, \ldots, f_{25}, f_{26}, f_{27}$$
$$f_1^{eq}, f_2^{eq}, f_3^{eq}, f_4^{eq}, f_5^{eq}, \ldots, f_{25}^{eq}, f_{26}^{eq}, f_{27}^{eq}$$

Total values to store: 58,000,000

Often need more memory to store intermediate values

LBM	FEM + FVM
☐ Node-wise solving	☐ Essentially fancy linear algebra
☐ Highly parallelable	☐ Medium parallelable
☐ Models mesoscopic interactions	☐ Models macroscopic evolution
☐ Weakly incompressible	☐ Strongly incompressible
☐ Local nonlinearity	☐ Global nonlinearity
☐ Confined to regular lattice	☐ Complex geometries with unstructured meshes

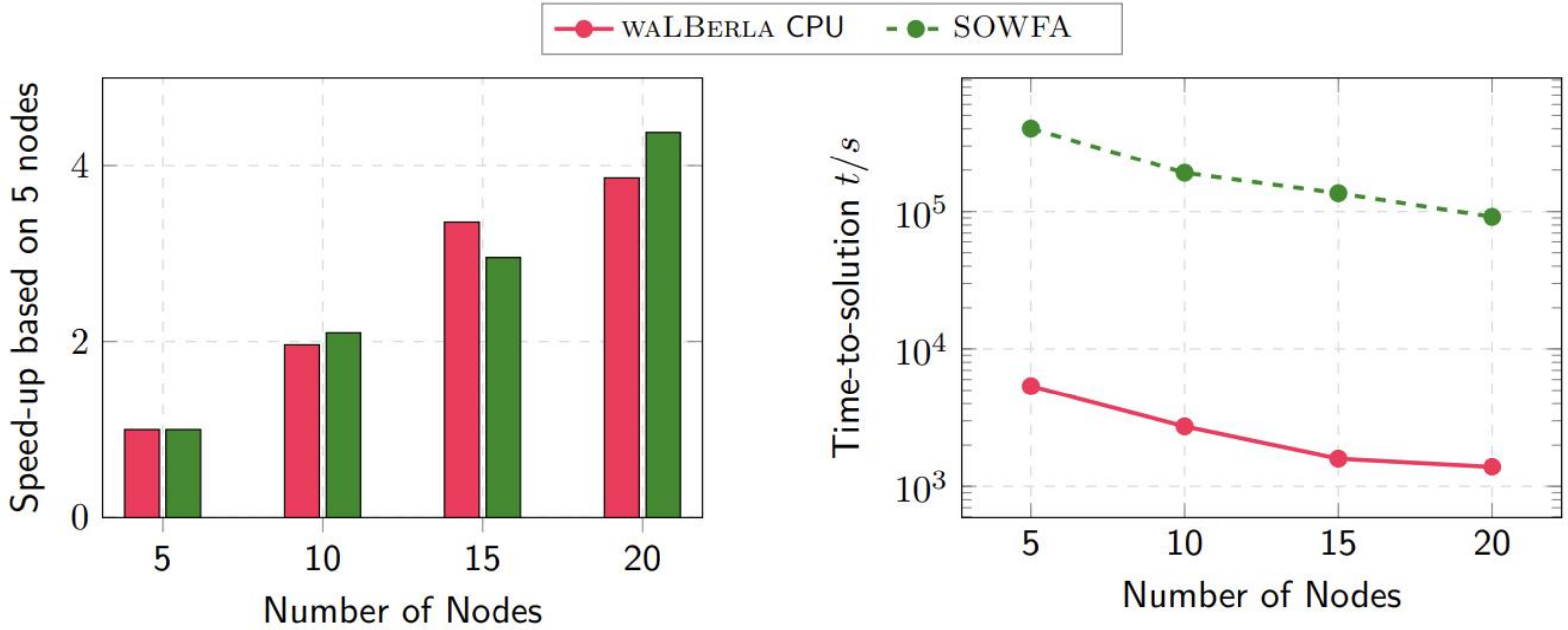
OpenLB

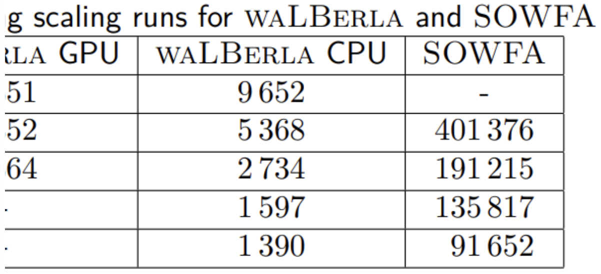


OpenLB – Open Source Lattice Boltzmann Code

The OpenLB project provides a C++ package for the implementation of lattice Boltzmann methods that is general enough to address a vast range of transport problems, e.g. in computational fluid dynamics. The source code is publicly available and constructed in a well readable, modular way. This enables for a fast implementation of both academic and advanced engineering applications. It is also easily extensible to include new physical models.

Speed Of LBM-ALM




g scaling runs for waLBerla and SOWFA

LA GPU	waLBerla CPU	SOWFA
51	9 652	-
52	5 368	401 376
64	2 734	191 215
-	1 597	135 817
-	1 390	91 652

enhamml et al 2022]

Figure 5. Strong scaling experiment with $163\,840\,000$ cells, $1\,200s$ simulated physical time with $\Delta t = 0.026s$: Speed-up based on the simulation time on five nodes (left), performance in time-to-solution (right)

Dissipative LBM

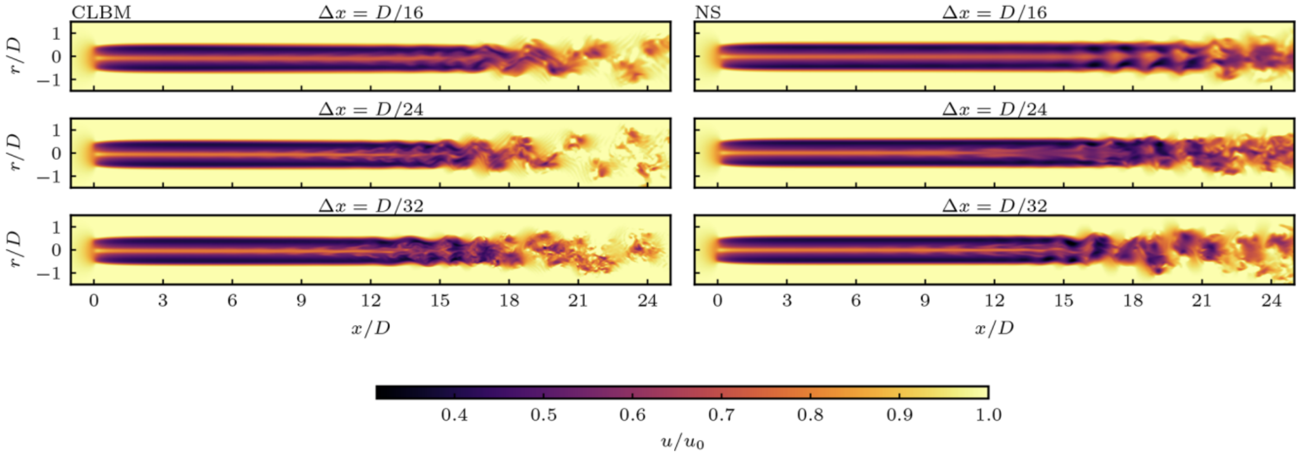


Figure 7. Contour plots of the instantaneous stream-wise velocity u in the central stream-wise plane at different spatial resolutions (top to bottom panels) with the CLBM (left panels) and NS (right panels).

[Asmuth et al 2020]