

EGEE 520: Mathematical Modeling Lattice-Boltzmann Method

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Introduction

Transport equations (for heat, mass, momentum) can be simulated on different scales.



Micro-Scale

- Models each individual particle
- Behavior governed by Hamilton's equation
- Too much data to handle in order to simulate a problem that is interesting.
 - Would need to know position and velocity of each molecule
 - One liter of air contains 10^{22} molecules

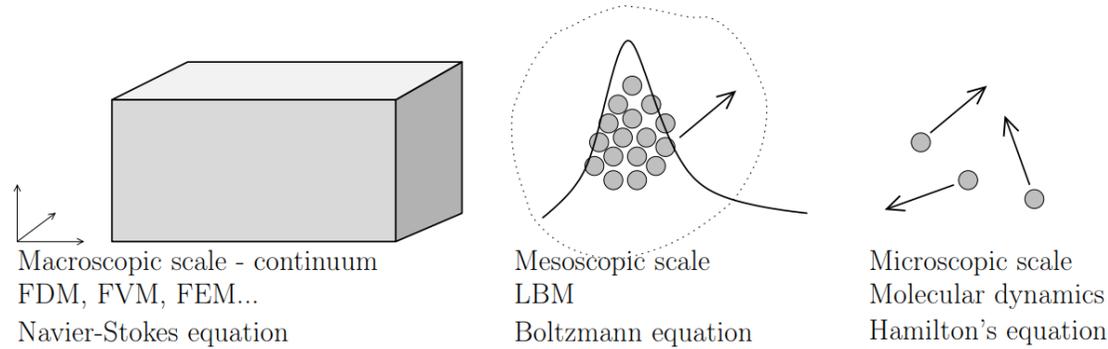
Macro-Scale

- Partial differential equations (PDE) such as Navier-Stokes are used
- Can be solved using numerical schemes
 - Finite Difference Method (FDM)
 - Finite Volume Method (FVM)
 - Finite Element Method (FEM)

1 Introduction

Where does Lattice-Boltzmann Method lie?

- Lattice-Boltzmann method is used to model on a scale that lies between micro and macro which is called mesoscopic scale.



- Considers the behavior of a collection of particles as a unit
- LBM is based on microscopic models and mesoscopic kinetic equations
- The property of the collection of particles is represented by a distribution function that is derived from the Boltzmann equation

Image source: Igor Mele

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Introduction

The Differences

Navier-Stokes equation	Lattice Boltzmann equation
$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u}$	$\frac{\partial f}{\partial t} + \mathbf{e} \cdot \nabla f = -\frac{1}{\tau} (f - f^{\text{EQ}})$
second-order PDE	first-order PDE
need to treat the non-linear convective term $\mathbf{u} \cdot \nabla \mathbf{u}$	avoids convective term, convection becomes simple advection
need to solve Poisson equation for the pressure p	pressure p is obtained from equation of state

Table source: Igor Mele

1 Introduction

LBM Advantages

- Ideal for parallel computing since the solutions are localized and the problem can be broken down to be solved by multiple computers simultaneously (computational clusters)
- Can be applied to micro-scale fluid flow problems since the Boltzmann equation is kinetic-based and the physics associated with molecular level interactions can be incorporated more easily
- Complex geometry, physics, and flow phenomena is not an issue
- Can efficiently model multi-phase flow

1 Introduction

LBM Disadvantages

- High memory is required and in many cases, the memory access can be more time consuming than performing arithmetic operations
 - Modeling a problem with 8×8 points requires $8 \times 8 \times 9 = 576$ variables
- The time-dependent Lattice Boltzmann Method is inefficient for solving steady-state problems, because its speed of convergence is dictated by acoustic propagation, which is very slow
- Standard models only work with Mach numbers up to ~ 0.2
 - Largest pressure changes supported are of the order $\frac{\delta P}{P} \sim Ma^2$
 - Modeling larger pressure gradients requires modeling external forces
$$F_{ext} = -\nabla P$$

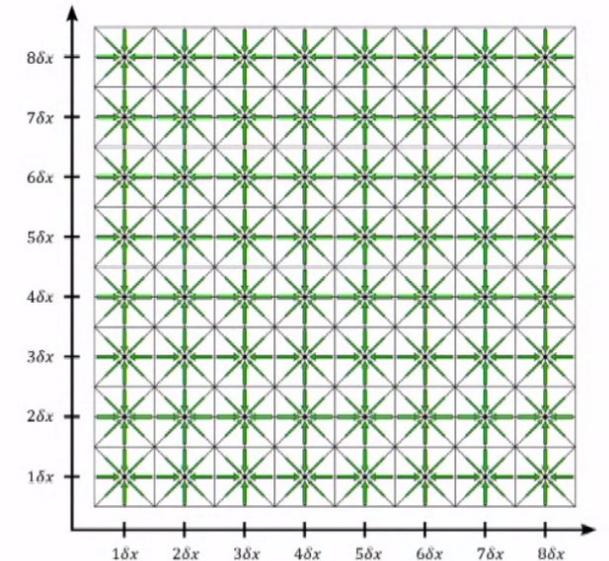


Image source: Bastien Chopard

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Historical Perspective: Overview

Fundamentals

- **Maxwell-Boltzmann Distribution (1860)**
- **Boltzmann Transport Equation (1872)**

Prototype Models

- **Broadwell (1964)**
- **Hardy, de Pazzis, and Pomeau (HPP) Model (1973)**

Lattice Boltzmann Methods (LBM)

- **McNamara & Zanetti (1988)**
- **Strumolo & Viswanathan (1997)**
- **Chen & Doolen (1998)**
- **Boon et al (1996)**
- **Zhong et al (2006)**

Lattice Gas Automata (LGA)

- **Frisch, Hasslacher, and Pomeau (1986) and Wolfram (1986)**
- **d'Humieries et al (1986)**



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Historical Perspective: Fundamentals

Maxwell-Boltzmann Distribution

- **Result of kinetic theory of gases**
 - **Applies to classical ideal gases**
- **Distribution of particle speeds indicates which speeds are more probable**
- **Derived heuristically by Boltzmann in 1860**

$$f(v) d^3v = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{m|v|^2}{2kT}} d^3v$$

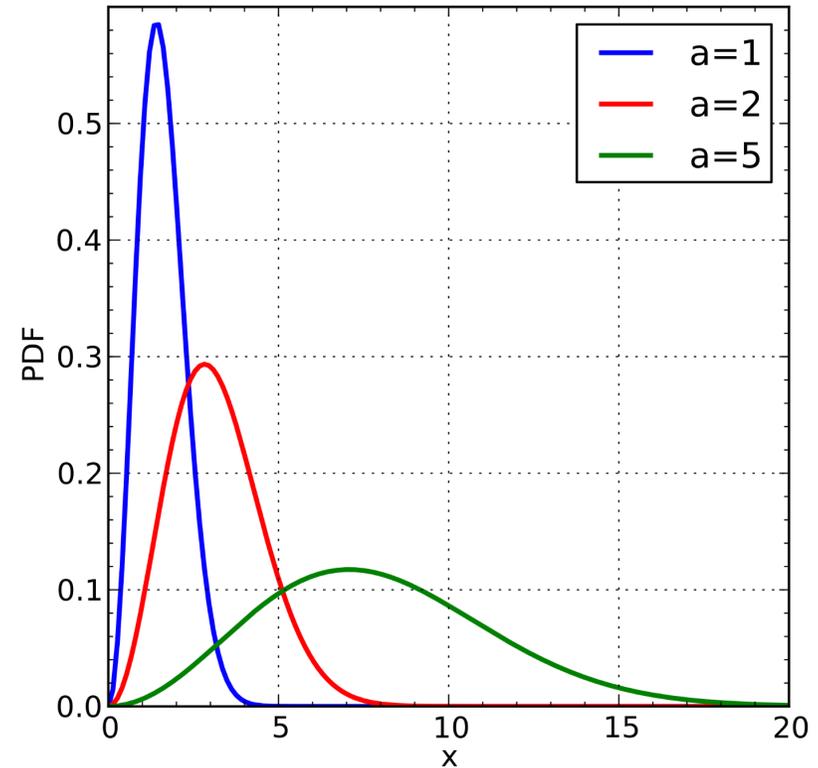


Image source: Krishnavedala

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Historical Perspective: Fundamentals

Boltzmann Transport Equation (1872)

- Considers probability distribution of position and momenta of particles rather than explicit positions and momenta
- Can determine how physical properties change (heat, momentum, energy) as well as fluid characteristics (viscosity, thermal conductivity)

Phase Space

$$d^3r d^3p = dx dy dz dp_x dp_y dp_z$$

Principal Statement

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{force} + \left(\frac{\partial f}{\partial t}\right)_{diff} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{F}{m} \cdot \frac{\partial f}{\partial v} = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

2

Historical Perspective: Prototype Models

- **Broadwell (1964)**
 - **Boltzmann equation was solved for a few discrete velocities to study aerodynamics**
 - **Molecular velocities restricted to eight equal speeds**
- **Hardy, de Pazzis, and Pomeau (HPP) Model (1973)**
 - **Square lattice**
 - **Particle movement restricted to four cells that share a common edge (no diagonal movement)**
 - **Lacked rotational invariance – highly anisotropic**

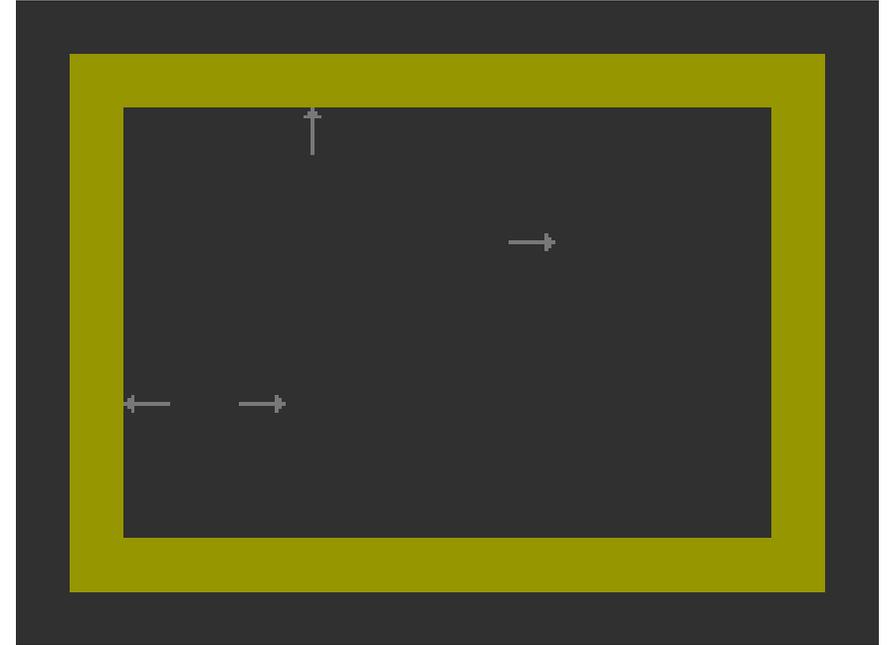


Image source: SimsContPics

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Historical Perspective: Lattice Gas Automata

- Hexagonal lattice
- Particles modeled with discrete velocities and can only move to other lattice nodes
- Boolean true/false variables to model whether or not a particle is at each lattice node
- Frisch, Hasslacher, and Pomeau (1986) and Wolfram (1986) proposed the first 2D LGA model for CFD
 - Reproduced correct Navier-Stokes equations
- d'Humieries et al (1986) introduced the first 3D model
- Problems with LGA:
 - Statistical noise from Boolean variables
 - Viscosity limitations – limited Re range
 - Potential unphysical solution due to simple symmetries in hexagonal grid

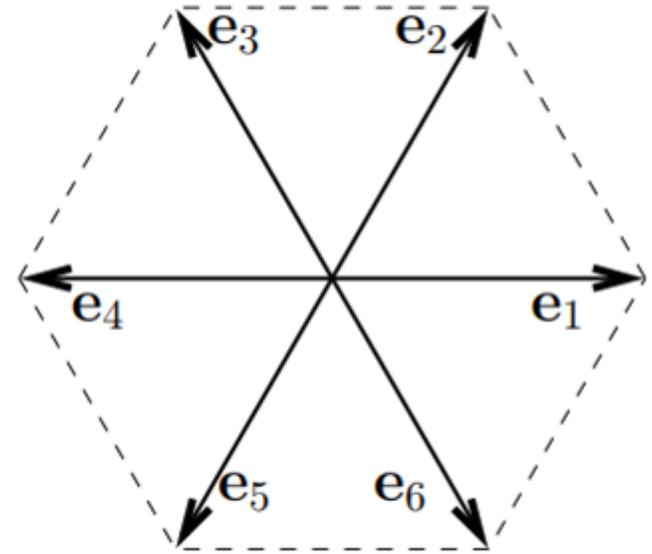
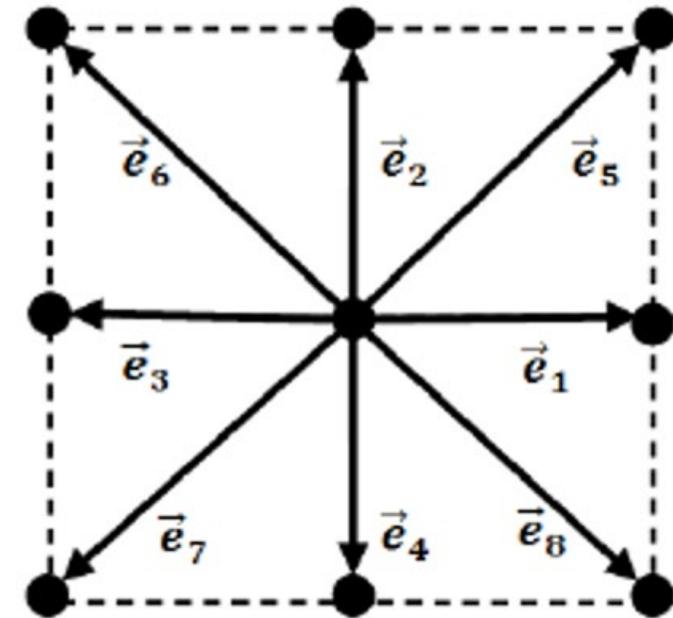


Image source: Bao & Meskas

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Fixed with Lattice Boltzmann Method!

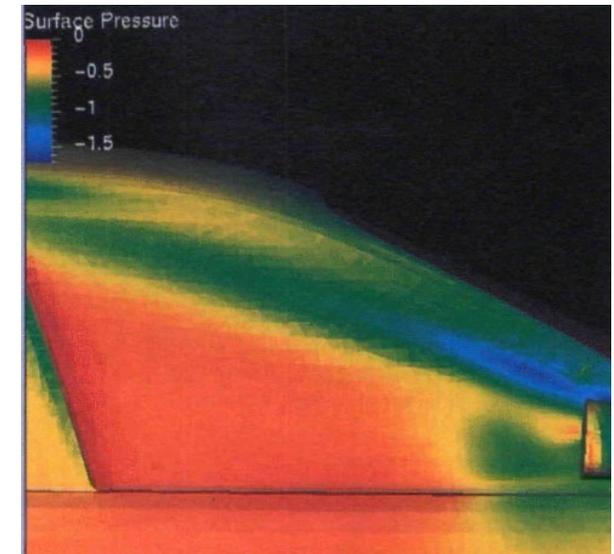
- 9 node square lattice with diagonal movement
- Boolean variables replaced with particle distribution function

Image source: Bao & Meskas

2 Historical Perspective: Lattice Boltzmann Method

Since its inception by McNamara & Zanetti in 1988, LBM techniques have been used to model many interesting physical situations

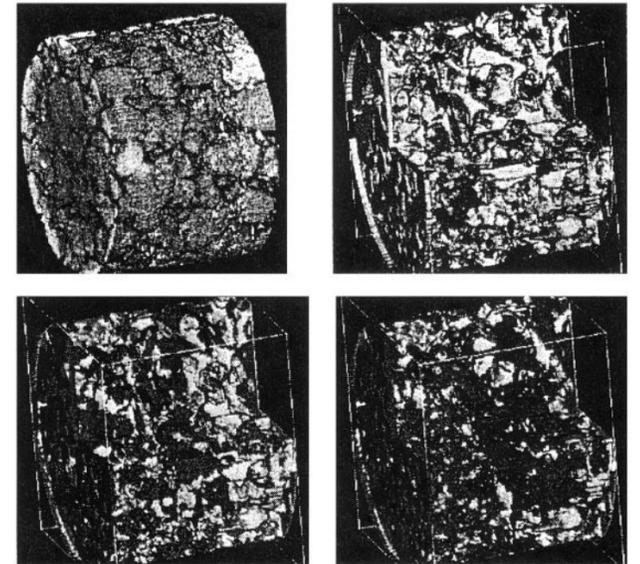
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 - **Turbulent external flow over structures with complicated boundaries (flow over a Ford Taurus)**
- **Chen & Doolen (1998)**
 - **Multi-phase, multi-component flow through porous media**
- **Boon et al (1996)**
 - **Chemical reactive flows**
- **Zhong et al (2006)**
 - **Simulation of the Schrödinger equation**



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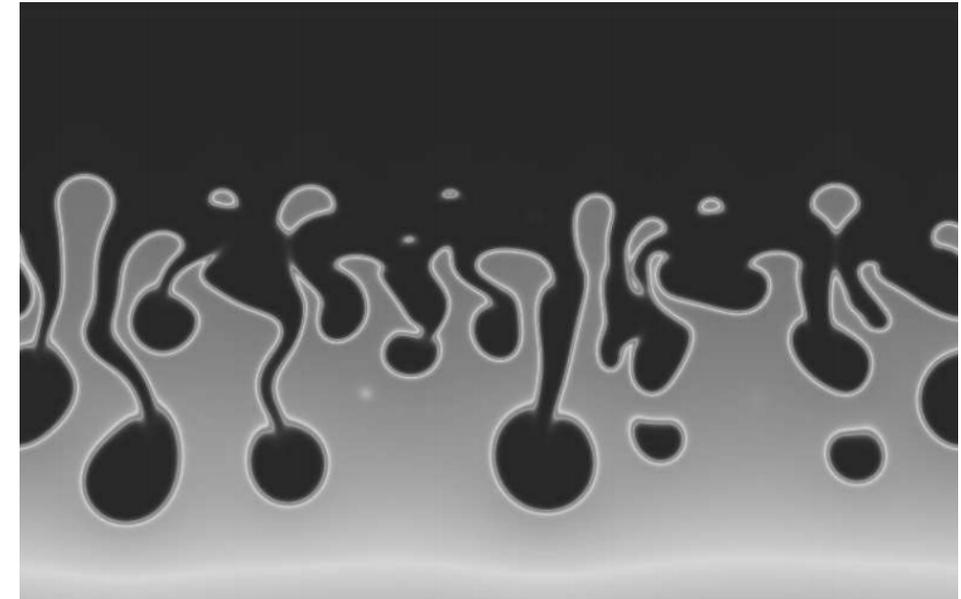
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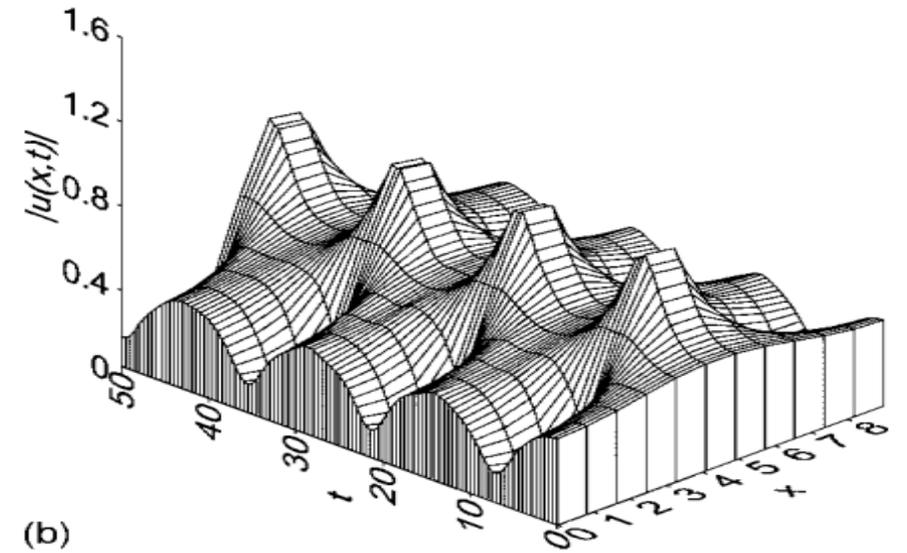
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3

General Principles: LGA Formulation

Local
particle
velocity

Collision operator

- -1 if particle destroyed
- 0 if particle unchanged
- 1 if particle created

$$n_i(x + e_i \delta t, t + 1) = n_i(x, t) + \Omega_i(n(x, t))$$

Boolean true/false

- 0 if no particle at location
- 1 if particle at location
- Two particles cannot occupy same node

3

General Principles: LGA Formulation

At each time step, the configuration of particles evolves in two sequential sub-steps

- **Streaming step**
 - Each particle moves to the nearest node in the direction of its velocity
- **Collision step**
 - Particles arrive at node and interact by changing their velocity direction according to scattering rules

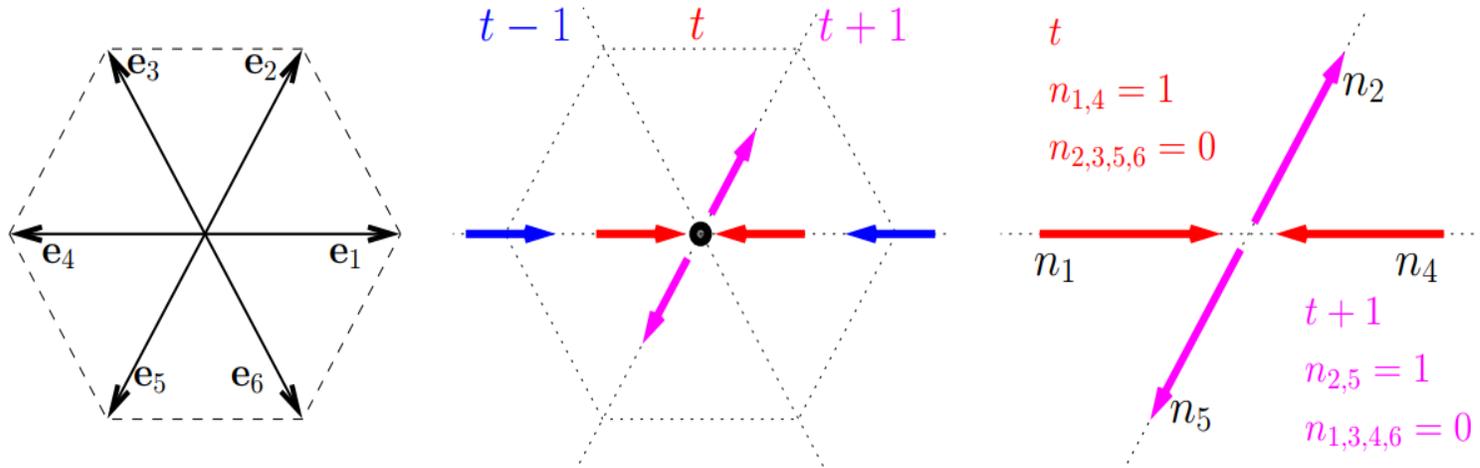


Image source: Bao & Meskas

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General Principles: LGA to LBM

Replace Boolean n_i values with single particle distribution functions, f_i

- f_i can be any value between 0 and 1
- $f(x, e, t)$ – distribution function depends on position vector x , velocity vector e , and time t
 - represents the number of particles with mass m at time t positioned between $x + dx$ which have velocities between $e + de$
 - After time dt , position and velocity values update such that
 - $x \rightarrow x + edt$
 - $e \rightarrow e + \frac{F}{m} dt$

This formulation simplifies Boltzmann's original idea of gas dynamics by reducing the number of particles and confining them to the nodes of a lattice

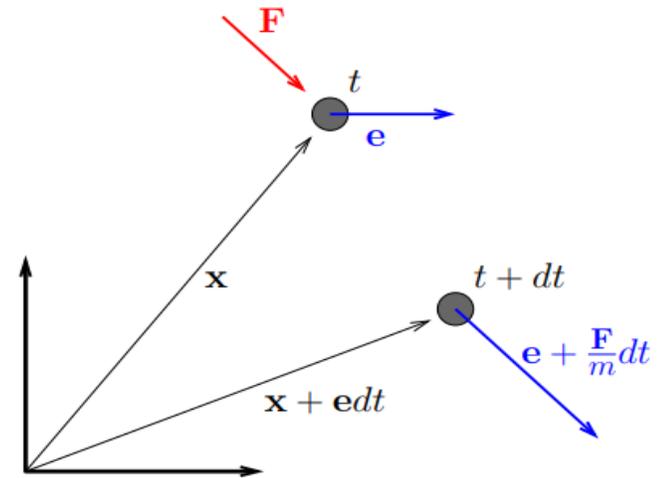
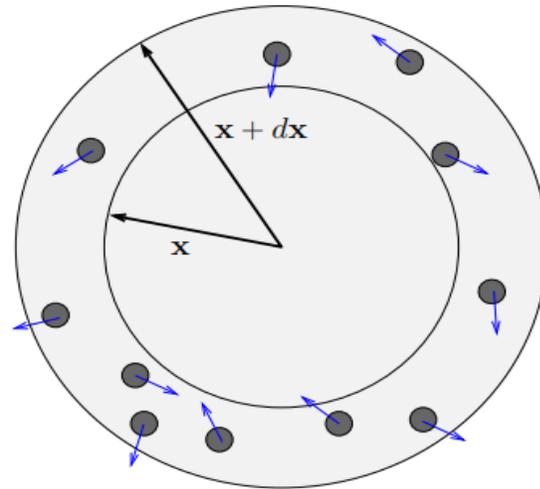


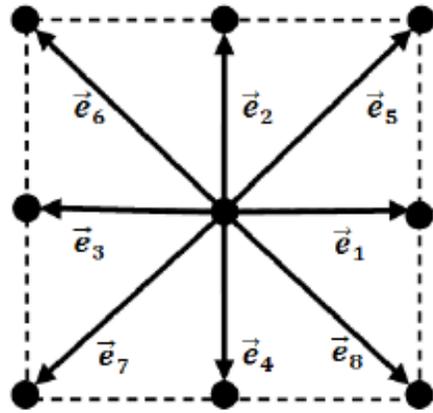
Image source: Igor Mele

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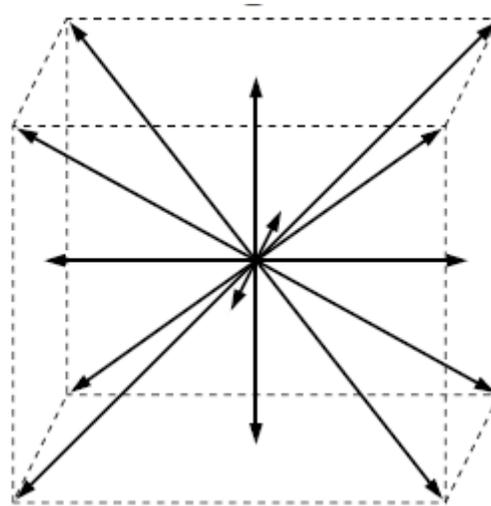
General Principles: Lattice Notation and Types

Many possible lattices can be modeled of the form D_nQ_m

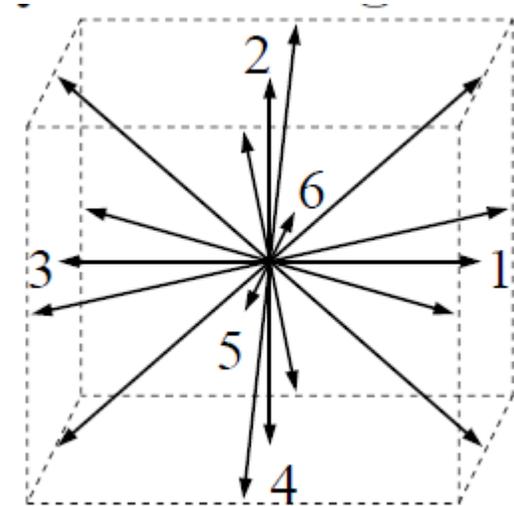
- Lattice has n spatial dimensions and m discrete velocities



D2Q9



D3Q15



D3Q19

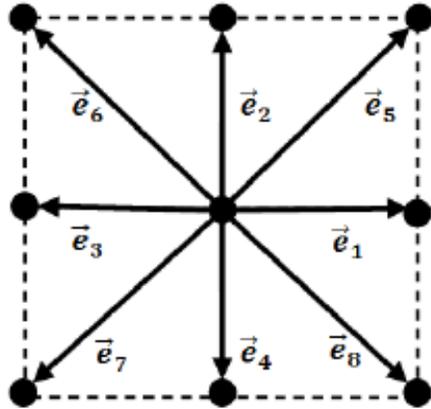
Image source: Alexander Wagner

3

General Principles: Lattice Notation and Types

Many possible lattices can be modeled of the form DnQm

- Lattice has n spatial dimensions and m discrete velocities



D2Q9

- D2Q9 lattice has two spatial dimensions and 9 discrete velocities
- Eight distribution functions f_i associated with particles moving to the neighboring cells and one distribution function f_i corresponding to the resting particles
- Discrete (microscopic) velocities are given by:

$$e_i = \begin{cases} (0,0), & i = 0 \\ (1,0), (0,1), (-1,0), (0,-1), & i = 1,2,3,4 \\ (1,1), (-1,1), (-1,-1), (1,-1), & i = 5,6,7,8 \end{cases}$$

Image source: Alexander Wagner

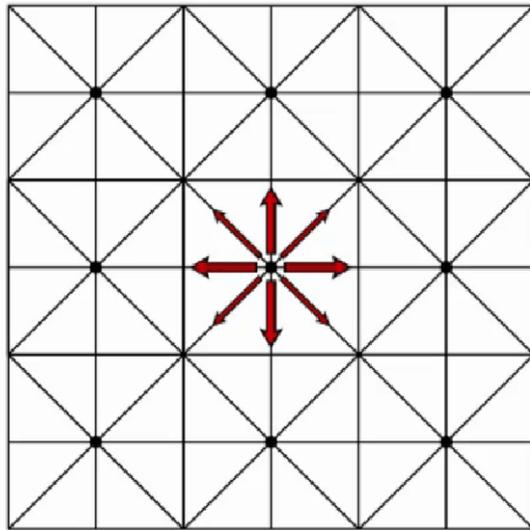
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General Principles: Streaming and Collision

At each time step, the configuration of particles evolves in two sequential sub-steps (same idea as in LGA)

Streaming step

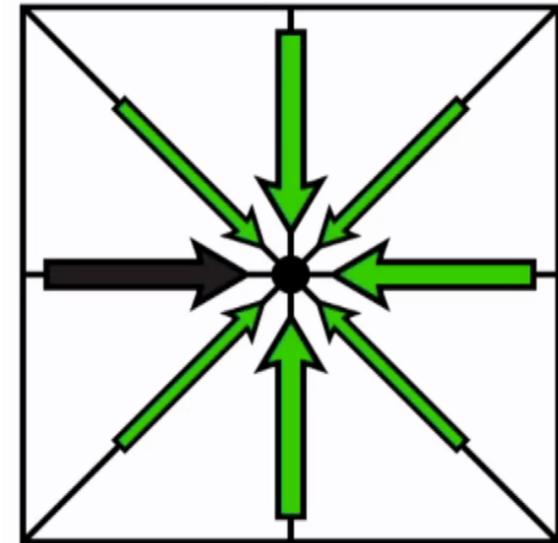
Each particle moves to the nearest node in the direction of its velocity



$$t \rightarrow t + \delta t$$

Collision step

Particles arrive at node and interact by changing their velocity direction according to scattering rules



Animation source: Bastien Chopard



4 Governing Equations: Problem Formulation

Begin with result from Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{F}{m} \cdot \frac{\partial f}{\partial v} = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

Neglecting external forces (when is this assumption valid?), we get that

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

- Note that v is macroscopic velocity, whereas e is discrete particle velocity

4

Governing Equations: Collision Operator

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

$\left(\frac{\partial f}{\partial t} \right)_{coll}$, the collision operator, is generally a complex, non-linear integral. To simplify this term, we use the Bhatnagar, Gross, Krook (BGK) operator model:

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = -\frac{1}{\lambda} (f - f^{eq})$$

Maxwell-Boltzmann equilibrium distribution function

Relaxation time

- BGK operator is valid (conserves mass and momentum) for single-phase flow where Mach number is small ($Ma \leq 0.2$)

4

Governing Equations: Collision Operator

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{1}{\lambda}(f - f^{eq})$$

For the BGK model, f_i^{eq} is defined as

$$f_i^{eq}(x, t) = w_i \rho + \rho s_i(v(x, t))$$

where $s_i(v)$ is defined as

$$s_i(v) = w_i \left[3 \frac{e_i \cdot v}{c} + \frac{9}{2} \frac{(e_i \cdot v)^2}{c^2} - \frac{3}{2} \frac{v \cdot v}{c^2} \right]$$

For a D2Q9 Lattice, common values chosen for w_i are

$$w_i = \begin{cases} \frac{4}{9}, & i = 0 \\ \frac{1}{9}, & i = 1, 2, 3, 4 \\ \frac{1}{36}, & i = 5, 6, 7, 8 \end{cases}$$

$$f_i^{eq} = \rho w_i \left[1 + 3 \frac{e_i \cdot v}{c} + \frac{9}{2} \frac{(e_i \cdot v)^2}{c^2} - \frac{3}{2} \frac{v \cdot v}{c^2} \right]$$

Lattice speed $c = \frac{\Delta x}{\Delta t}$
where, generally,
 $\Delta x = \Delta t$

4

Governing Equations: Streaming and Collision

$$\tau = \frac{\lambda}{\Delta t}$$

Substituting the BGK operator for $\left(\frac{\partial f}{\partial t}\right)_{coll}$ and discretizing the Boltzmann transport equation, we get that

$$\underbrace{f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t)}_{\text{Streaming}} = - \underbrace{\frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)]}_{\text{Collision}}$$

Streaming

Collision

Usually broken
into two steps:

$$f_i(x + e_i, t + \Delta t) = f_i^*(x, t)$$

$$f_i^*(x, t) = f_i(x, t) - \frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)]$$



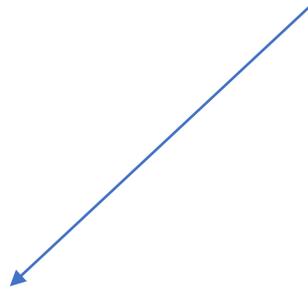
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Governing Equations: Streaming and Collision

$$\tau = \frac{\lambda}{\Delta t}$$

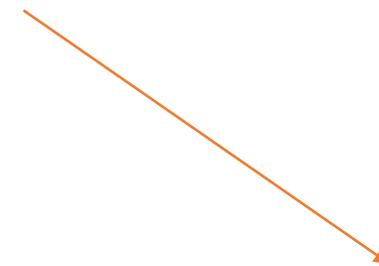
In these equations, f_i^* is the distribution of values after collision (but before propagation) and f_i are the values after collision and propagation, with $f_i(x + e_i, t + \Delta t)$ entering the neighboring cell as data for the next time step.

Streaming



$$f_i(x + e_i, t + \Delta t) = f_i^*(x, t)$$

Collision



$$f_i^*(x, t) = f_i(x, t) - \frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)]$$

Usually broken
into two steps:

4 Governing Equations: Macroscopic Calculations

From the Boltzmann equation, macroscopic values for ρ and v can be calculated readily as

$$\rho(x, t) = \sum_{i=0}^N f_i(x, t)$$

$$v(x, t) = \frac{1}{\rho(x, t)} \sum_{i=0}^N e_i f_i(x, t)$$

4 Governing Equations: Bounce-back Boundary Conditions

- Macroscopically equivalent to no-slip conditions at the boundary
- In numerical applications, one should use a Boolean mask for the boundary and interior nodes.

The boundary of the fluid domain is aligned with the lattice points and the incoming directions of the distribution functions are reversed when encountering a boundary node, such that

$$f_i(x + e_i, t + \Delta t) = f_i^*(x, t) = f_{\bar{i}}(x, t)$$

with $e_{\bar{i}} = -e_i$ and $f_{\bar{i}}(x, t) = f(x, e_{\bar{i}}, t) = f(x, -e_i, t)$.

This BC effectively rotates the distribution functions on the node and thus they return back to the fluid with opposite momentum in the next time step. This results in zero velocities at the wall and ensures that there is no flux across the wall.

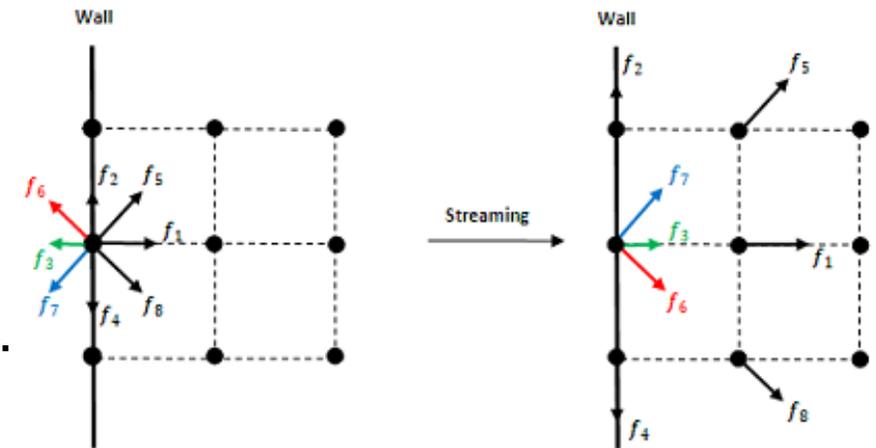
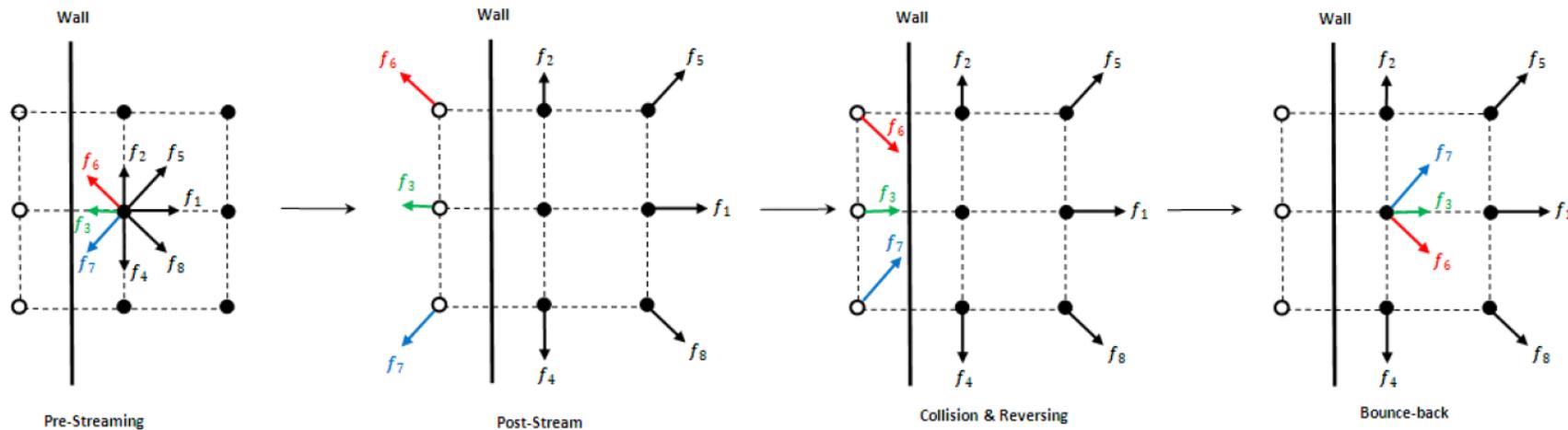


Image source: Bao & Meskas

4 Governing Equations: Bounce-back Boundary Conditions

There are also mid-grid bounce back boundary conditions in addition to those just discussed (on-grid bounce back boundary conditions)



- Introduces fictitious nodes and places the boundary wall centered between fictitious nodes and boundary nodes of the fluid
- Leads to second order accuracy, whereas on-grid bounce back is first order

Image source: Bao & Meskas

4 Governing Equations: Zou-He Boundary Conditions

Used to prescribe velocity or density at the boundary

In the case where a velocity is prescribed at the left boundary, after streaming, we have that $f_0, f_2, f_3, f_4, f_6,$ and f_7 are known.

With Zou-He BCs, we want to form a linear system of our unknowns $f_1, f_5, f_8,$ and ρ :

$$f_1 + f_5 + f_8 = \rho - (f_0 + f_2 + f_4 + f_3 + f_6 + f_7)$$

$$f_1 + f_5 + f_8 = \rho v_x + (f_3 + f_6 + f_7)$$

$$f_5 - f_8 = \rho v_y - f_2 + f_4 - f_6 + f_7$$

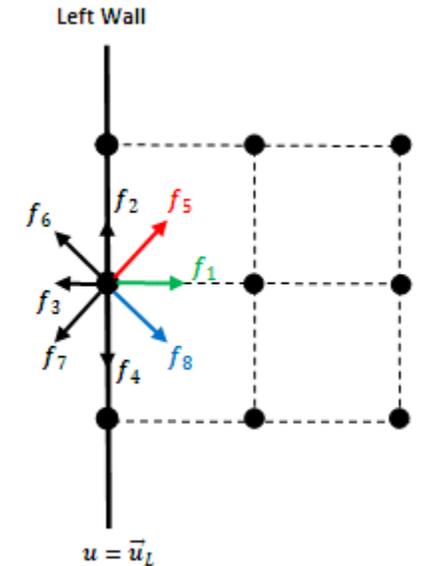


Image source: Bao & Meskas

4 Governing Equations: Zou-He Boundary Conditions

We can solve these equations to get

$$\rho = \frac{1}{1 - v_x} [f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)]$$

To close the system, we assume that the bounce-back rule holds for the non-equilibrium part of the particle distribution normal to the boundary, such that

$$f_1 - f_1^{eq} = f_3 - f_3^{eq}$$

Thus, we get that

$$\begin{aligned} f_1 &= f_3 + \frac{2}{3} \rho v_x \\ f_5 &= f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x + \frac{1}{2} \rho v_y \\ f_8 &= f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x - \frac{1}{2} \rho v_y \end{aligned}$$

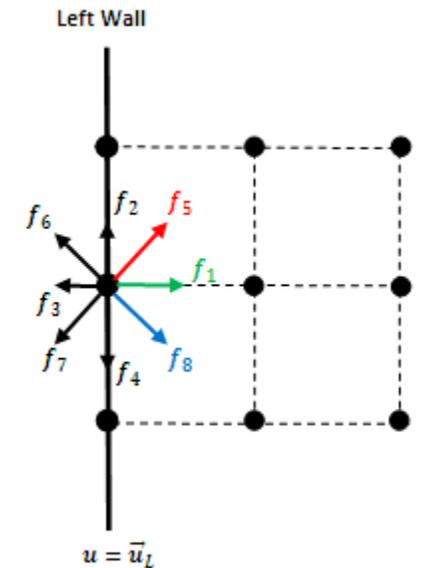


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4 Governing Equations: Summary of LBM Algorithm

Initialize Variables:

ρ, v, f_i



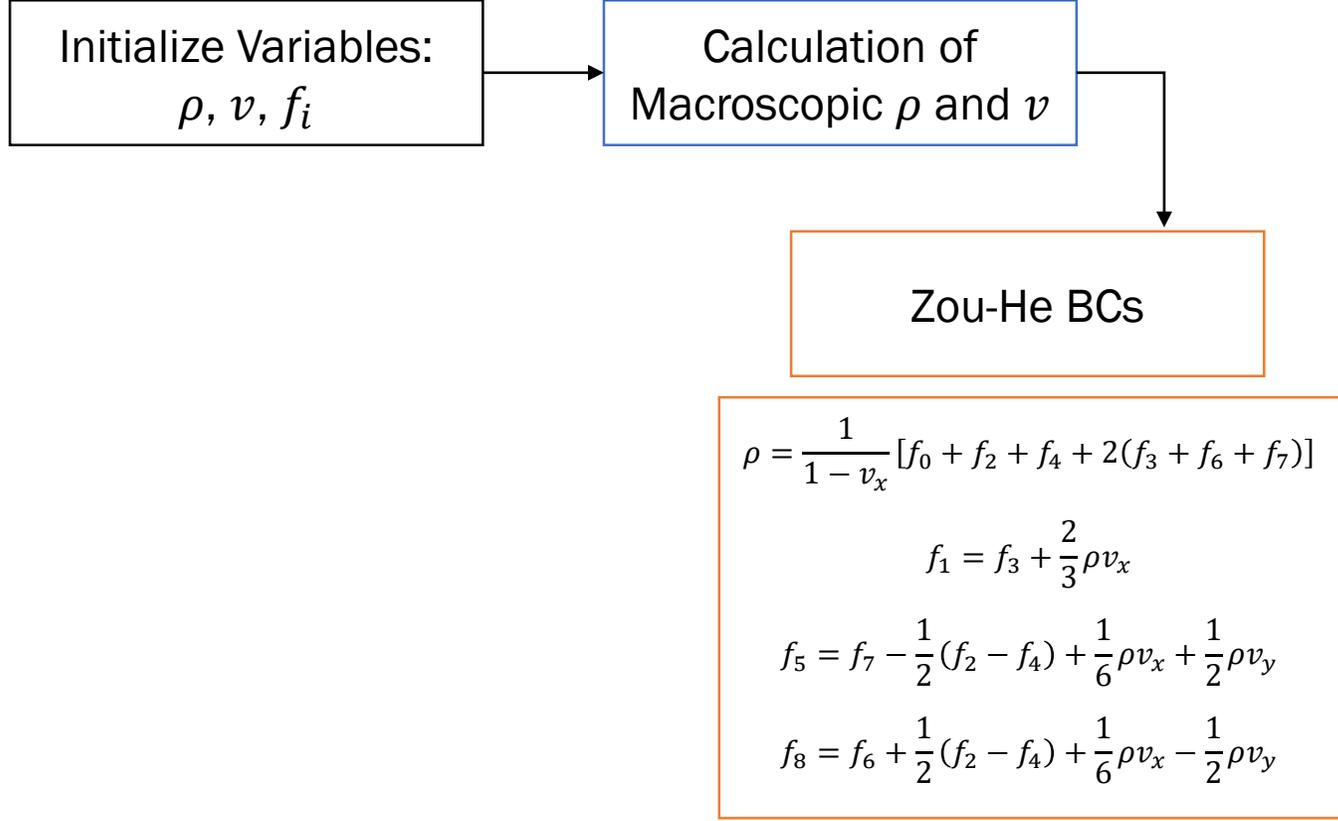
4 Governing Equations: Summary of LBM Algorithm

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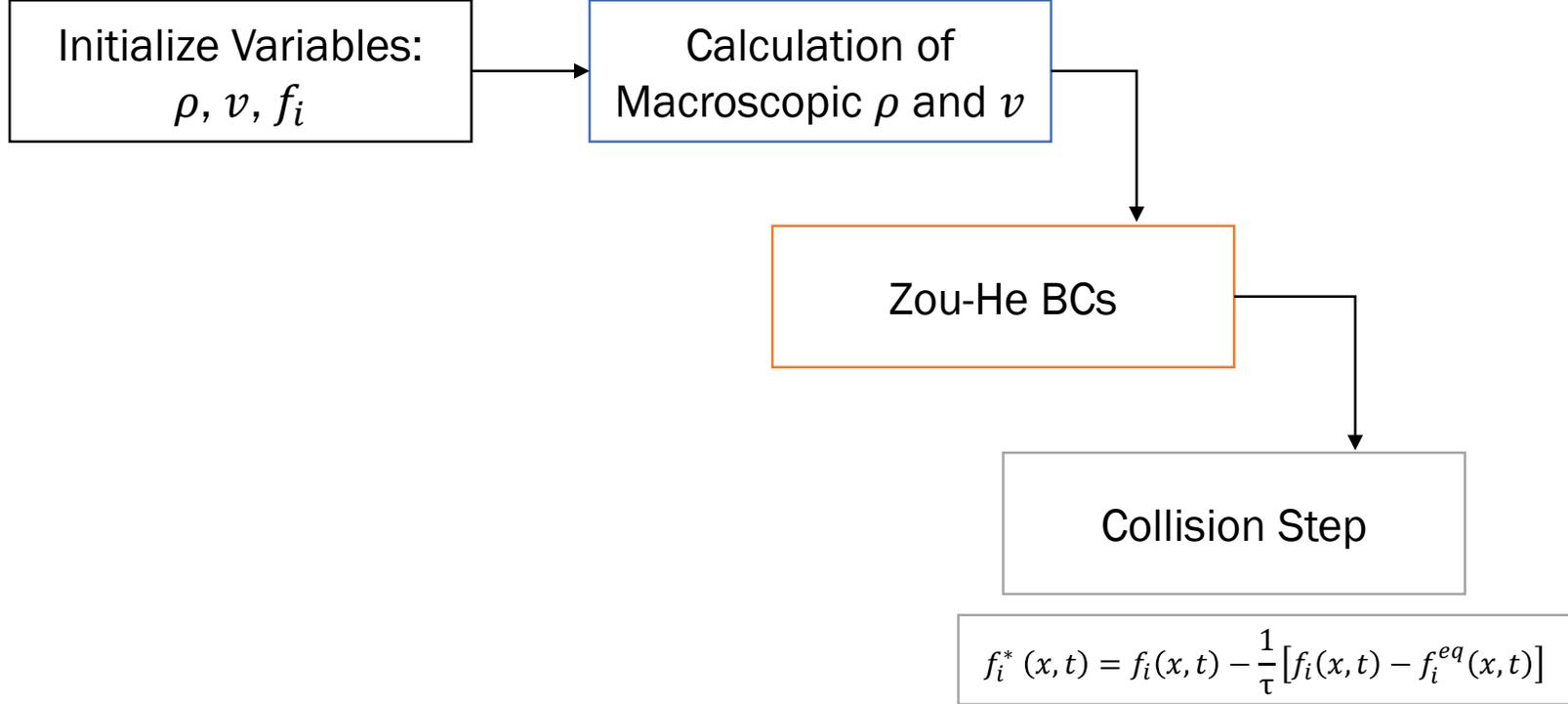
Calculation of
Macroscopic ρ and v

$$\rho(x, t) = \sum_{i=0}^N f_i(x, t)$$
$$v(x, t) = \frac{1}{\rho(x, t)} \sum_{i=0}^N e_i f_i(x, t)$$

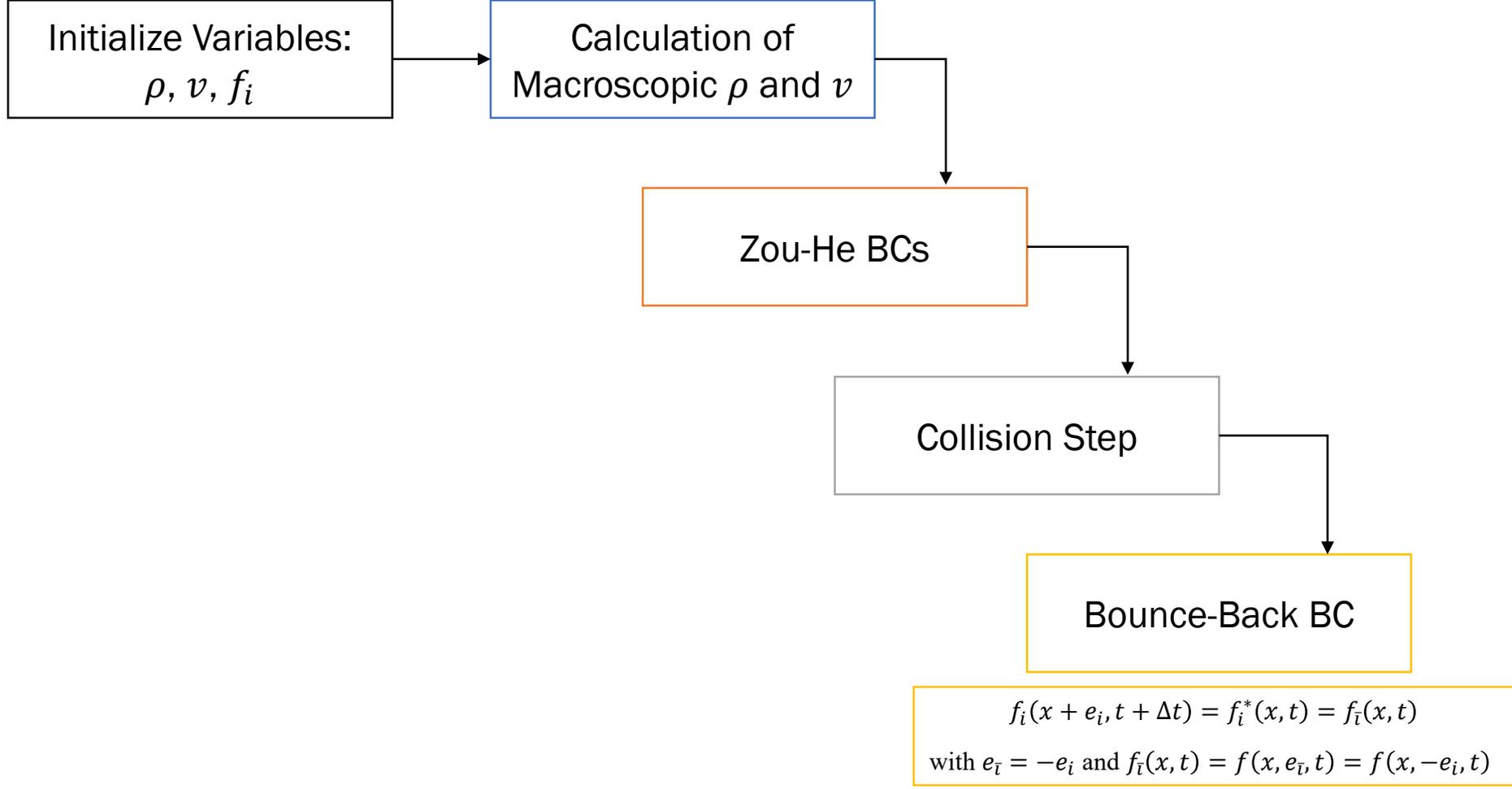
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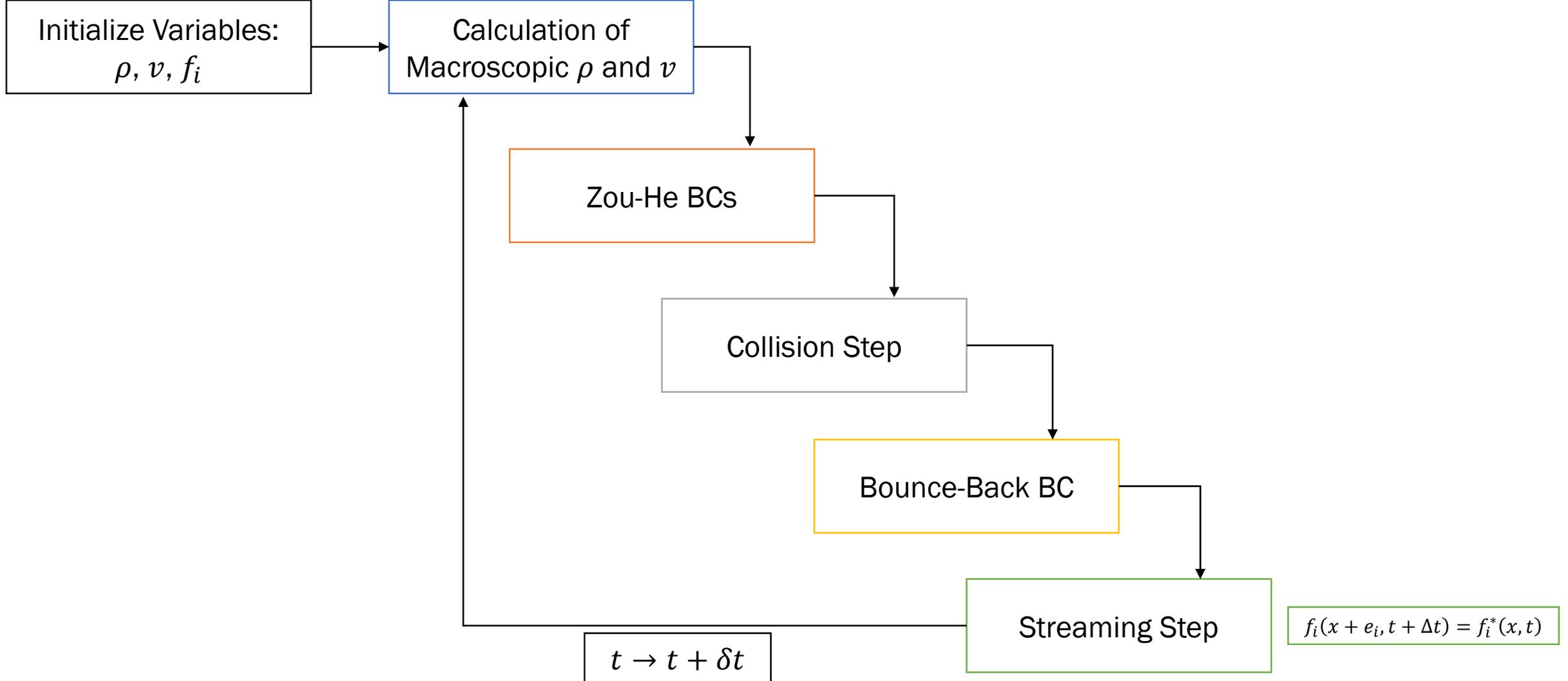
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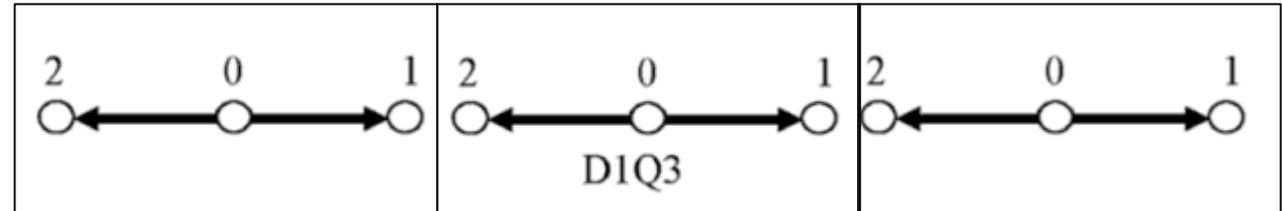
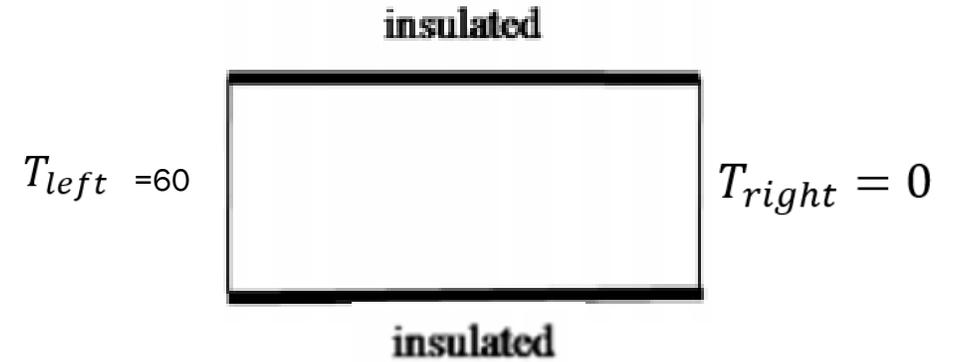
4 Governing Equations: Summary of LBM Algorithm



5

Hand Calculation: Problem Formulation

- D1Q3 model
- $T_{left} = 60, T_{right} = T_{middle} = 0$ | Boundary Conditions: bounce back
- Initial Conditions:
- $\rho = 1.0, \tau = 2.0, \delta t = 1.0$



Problem: Calculate the change in T as a function of time throughout the length of the pipe.

5

Hand Calculation: Initialization

Each element has 3 nodes

Weight Factors:

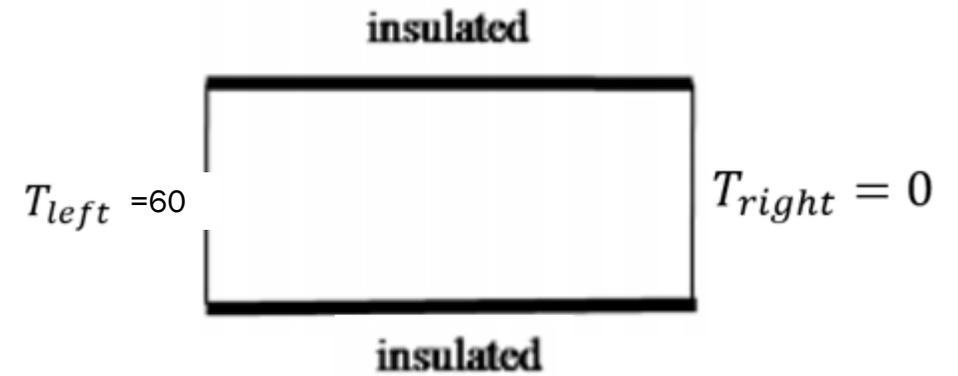
- $w_0 = 0.5, w_1 = w_2 = 0.25$

Distribution Function:

- $c_0 = 0, c_1 = 1, c_2 = -1$

$$f_i^{eq}(x, t) = w_i T(x, t)$$

- Where $T(x, t) = \sum f_i(x, t)$

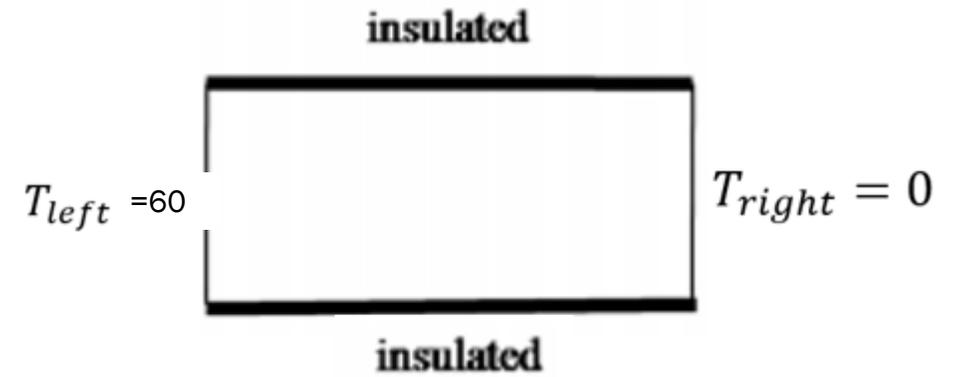


CELL A	CELL B	CELL C
F0= 30	F0=0	F0=0
F1=15	F1=60	F1=60
F2=15	F2=-60	F2=-60
$T(a, t) = \sum F_i = 60$	$T(b, t) = \sum F_i = 0$	$T(c, t) = \sum F_i = 0$
Equilibrium Distribution Functions		
$f_0^{eq} = 30$	$f_0^{eq} = 0$	$f_0^{eq} = 0$
$f_1^{eq} = 15$	$f_1^{eq} = 0$	$f_1^{eq} = 0$
$f_2^{eq} = 15$	$f_2^{eq} = 0$	$f_2^{eq} = 0$

5

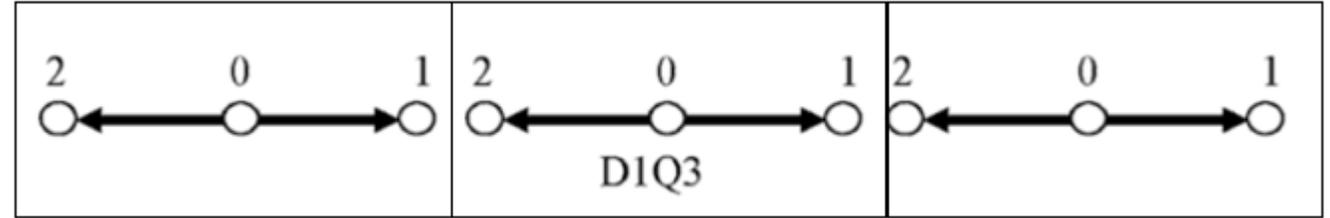
Hand Calculation: Collision

$$f_i^*(x, t) = (1 - \omega) f_i(x, t) + \omega f_i^{eq}(x, t)$$



BJK Approximation ← Collision Operator

Here, $\omega = \frac{\delta t}{\tau} = \frac{1}{2} = 0.5$



Sample Calculation for Cell A:

$$f_0^*(a, t) = (1 - 0.5) * 30 + 0.5 * 30 = 30$$

$$f_1^*(b, t) = (1 - 0.5) * 60 + 0 * 15 = 30$$

$$f_2^*(c, t) = (1 - 0.5) * -60 + 0 * 15 = -30$$

CELL A	CELL B	CELL C
$f_0^{eq} = 30$	$f_0^{eq} = 0$	$f_0^{eq} = 0$
$f_1^{eq} = 15$	$f_1^{eq} = 0$	$f_1^{eq} = 0$
$f_2^{eq} = 15$	$f_2^{eq} = 0$	$f_2^{eq} = 0$
Collision Term:		
$f_0^* = 30$	$f_0^* = 0$	$f_0^* = 0$
$f_1^* = 15$	$f_1^* = 30$	$f_1^* = 30$
$f_2^* = 15$	$f_2^* = -30$	$f_2^* = -30$

5

Hand Calculation: Streaming

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i^*(x, t)$$

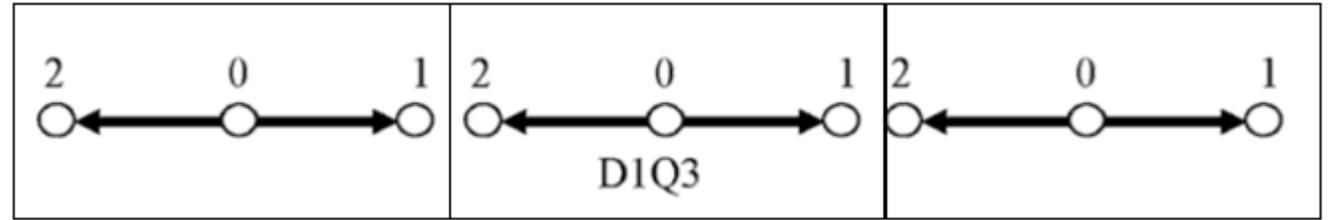
This step takes in account the B.C. applied to the system.

Sample Calculation:

$$f_0(a, t + dt) = f_0^*(a, t) = 30$$

$$f_1(b, t + dt) = f_1^*(a, t) = 15$$

$$f_2(c, t + dt) = f_2^*(b, t) = 15$$



CELL A	CELL B	CELL C
$f_0^{eq} = 30$ $f_1^{eq} = 15$ $f_2^{eq} = 15$	$f_0^{eq} = 0$ $f_1^{eq} = 0$ $f_2^{eq} = 0$	$f_0^{eq} = 0$ $f_1^{eq} = 0$ $f_2^{eq} = 0$
Collision Term:		
$f_0^* = 30$ $f_1^* = 15$ $f_2^* = 15$	$f_0^* = 0$ $f_1^* = 30$ $f_2^* = -30$	$f_0^* = 0$ $f_1^* = 30$ $f_2^* = -30$
Streaming Term:		
$f_0 = 30$ $f_1 = 15$ $f_2 = 15$ (B.C.)	$f_0 = 0$ $f_1 = 30$ $f_2 = -15$	$f_0 = 0$ $f_1 = 15$ (B.C.) $f_2 = -15$

$$*c_0 = 0, c_1 = 1, c_2 = -1$$

5

Hand Calculation: Update Macroscopic Distribution

Weight Factors:

$$w_0 = 0.5, w_1 = 0.25, w_2 = 0.25$$

Distribution Function:

$$c_0 = 0, c_1 = 1, c_2 = -1$$

$$f_i^{eq}(x, t) = w_i T(x, t)$$

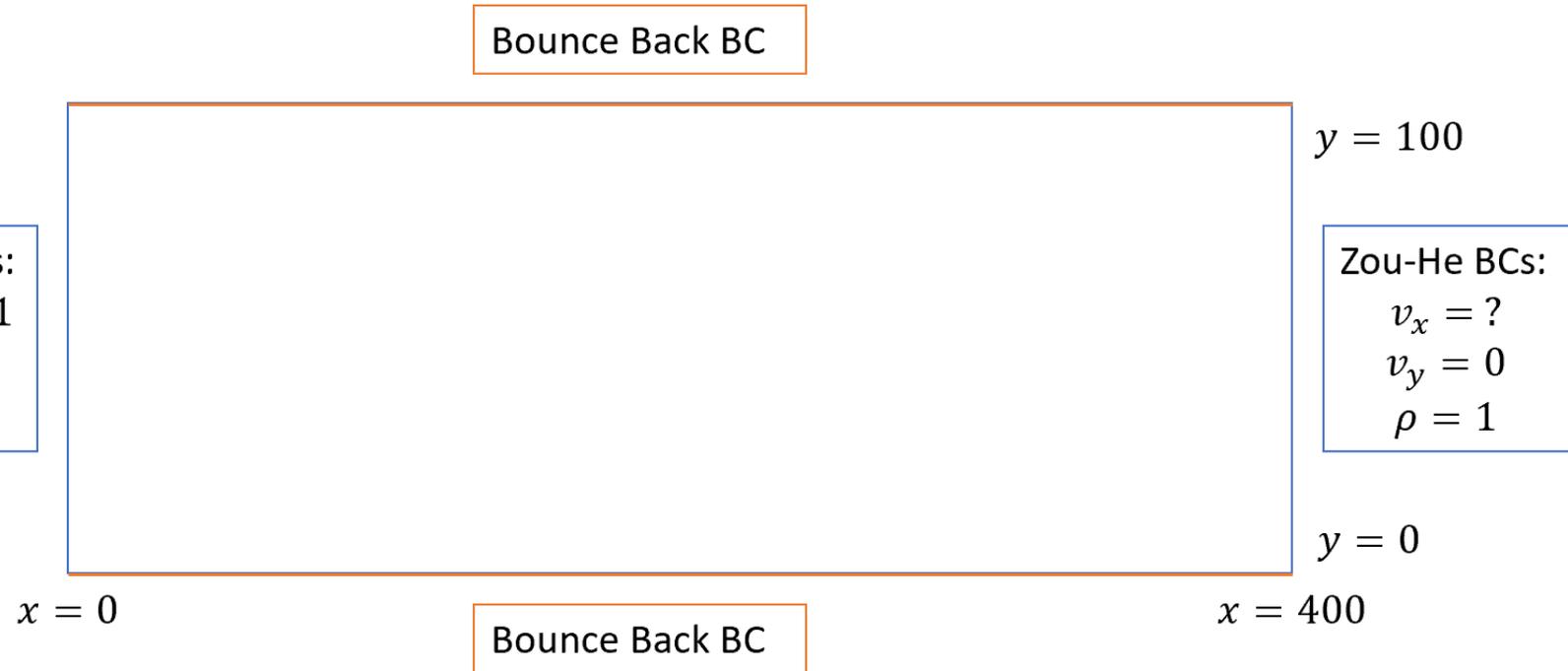
CELL A	CELL B	CELL C
Streaming Term:		
$f_0 = 30$ $f_1 = 15$ $f_2 = 15$ (B.C.)	$f_0 = 0$ $f_1 = 30$ $f_2 = -15$	$f_0 = 0$ $f_1 = 15$ (B.C.) $f_2 = -15$
$\sum f_i = 60$	$\sum f_i = 15$	$\sum f_i = 0$
Equilibrium Term for $t + \delta t: w_i * \sum F_i$		
$f_0^{eq} = 30$ $f_1^{eq} = 15$ $f_2^{eq} = 15$	$f_0^{eq} = 7.5$ $f_1^{eq} = 3.75$ $f_2^{eq} = 3.75$	$f_0^{eq} = 0$ $f_1^{eq} = 0$ $f_2^{eq} = 0$

6

Numeric Example: Case 1 – Prescribed Rate (Inlet), Prescribed Density (Outlet)

ICs:
 $v_x = 0.1$
 $v_y = 0$
 $\rho = 1$

Zou-He BCs:
 $v_x = 0.001$
 $v_y = 0$
 $\rho = ?$



6

Numerical Example: Code for Problem Formulation

Initialize Variables:

ρ, v, f_i

```
% D2Q9 LATTICE CONSTANTS
t = [4/9,1/9,1/9,1/9,1/9,1/36,1/36,1/36,1/36];
ex = [0,1,0,-1,0,1,-1,-1,1];
ey = [0,0,1,0,-1,1,1,-1,-1];
opp = [1,4,5,2,3,8,9,6,7];

% INITIAL CONDITION:
vx = 0.1*ones(lx,ly);
vy = zeros(lx,ly);
rho = 1;

for i=1:9
    cu = 3*(ex(i)*vx+ey(i)*vy);
    fIn(i, :, :) = rho .* t(i) .* ...
        ( 1 + cu + 1/2*(cu.*cu) - 3/2*(vx.^2+vy.^2) );
end
```

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6

Numerical Example: Code for Problem Formulation

Initialize Variables:
 ρ, v, f_i

Calculation of
Macroscopic ρ and v

```
% MACROSCOPIC VARIABLES  
rho = sum(fIn);  
vx = reshape ( (ex * reshape(fIn,9,lx*ly)), 1,lx,ly) ./rho;  
vy = reshape ( (ey * reshape(fIn,9,lx*ly)), 1,lx,ly) ./rho;
```

Palabos

CFD, COMPLEX

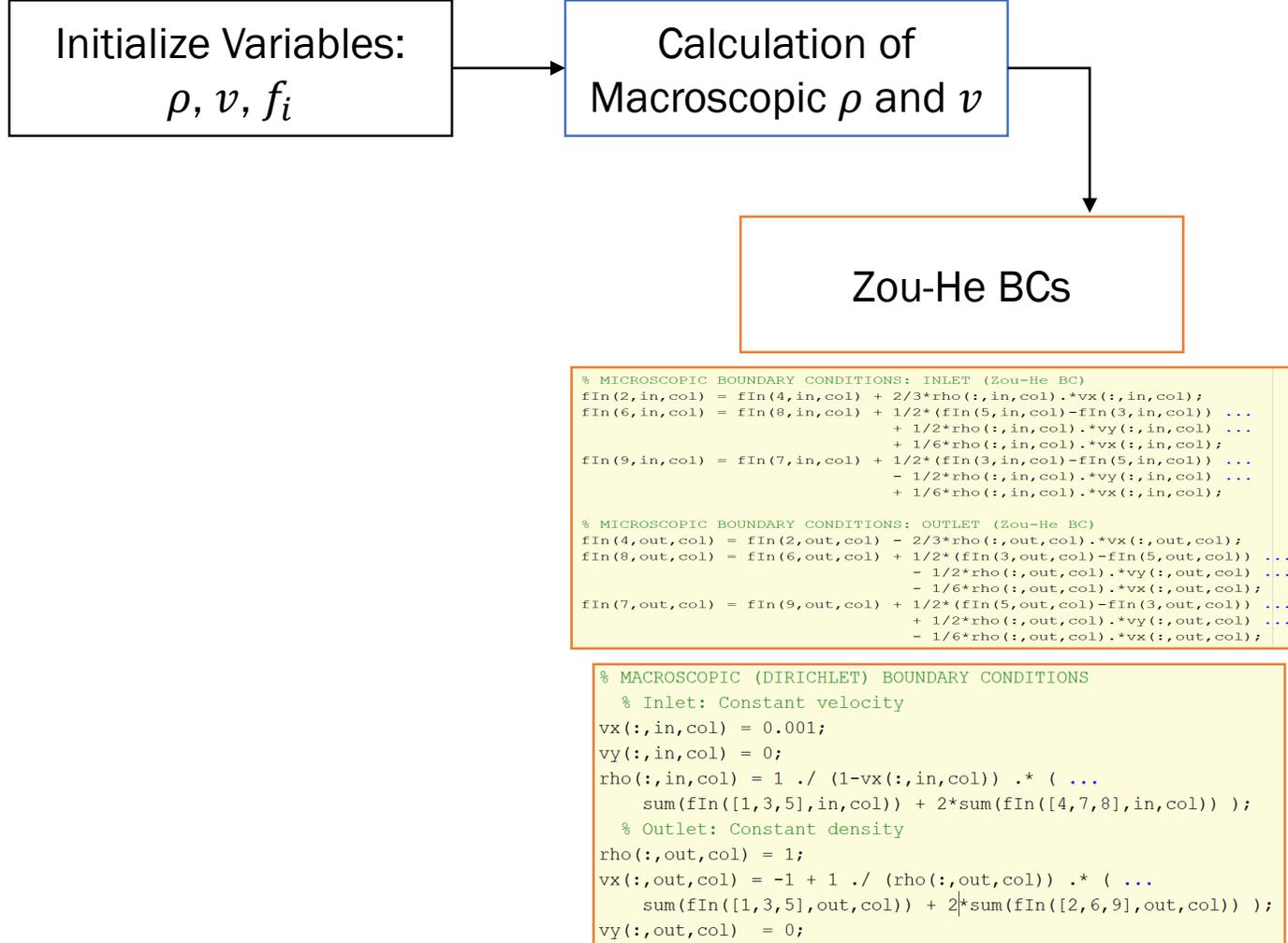
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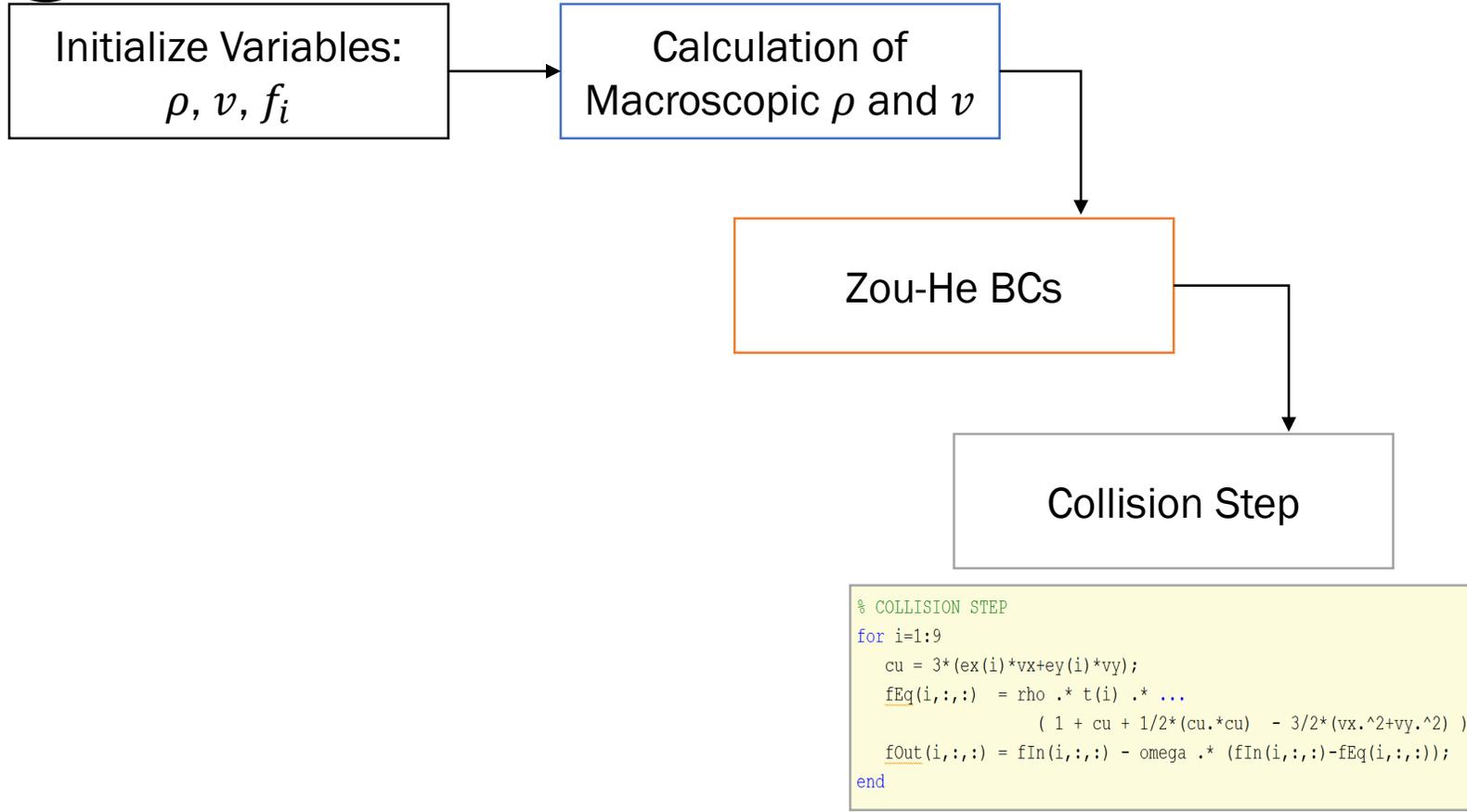
6

Numerical Example: Code for Problem Formulation



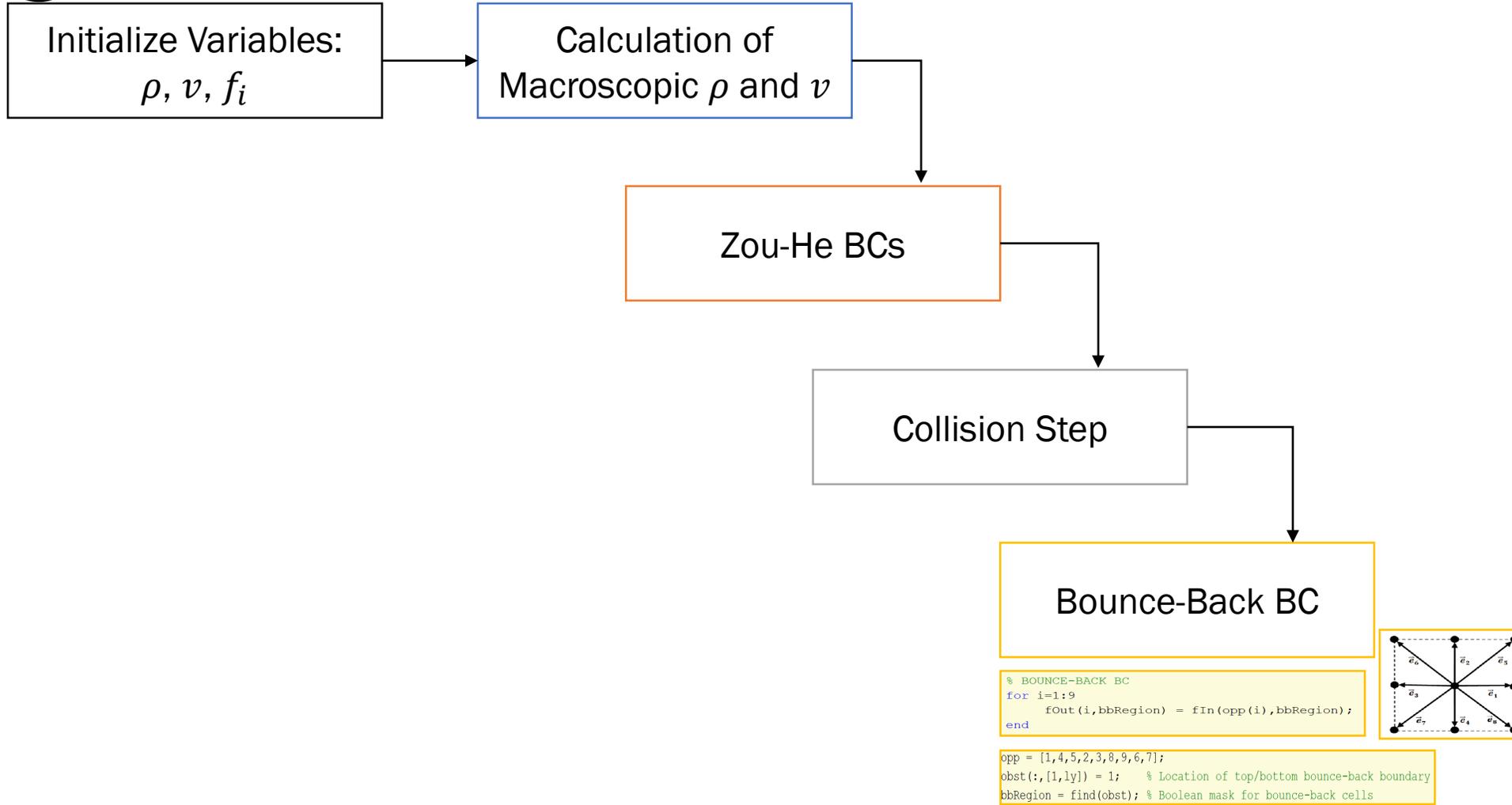
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Numerical Example: Code for Problem Formulation



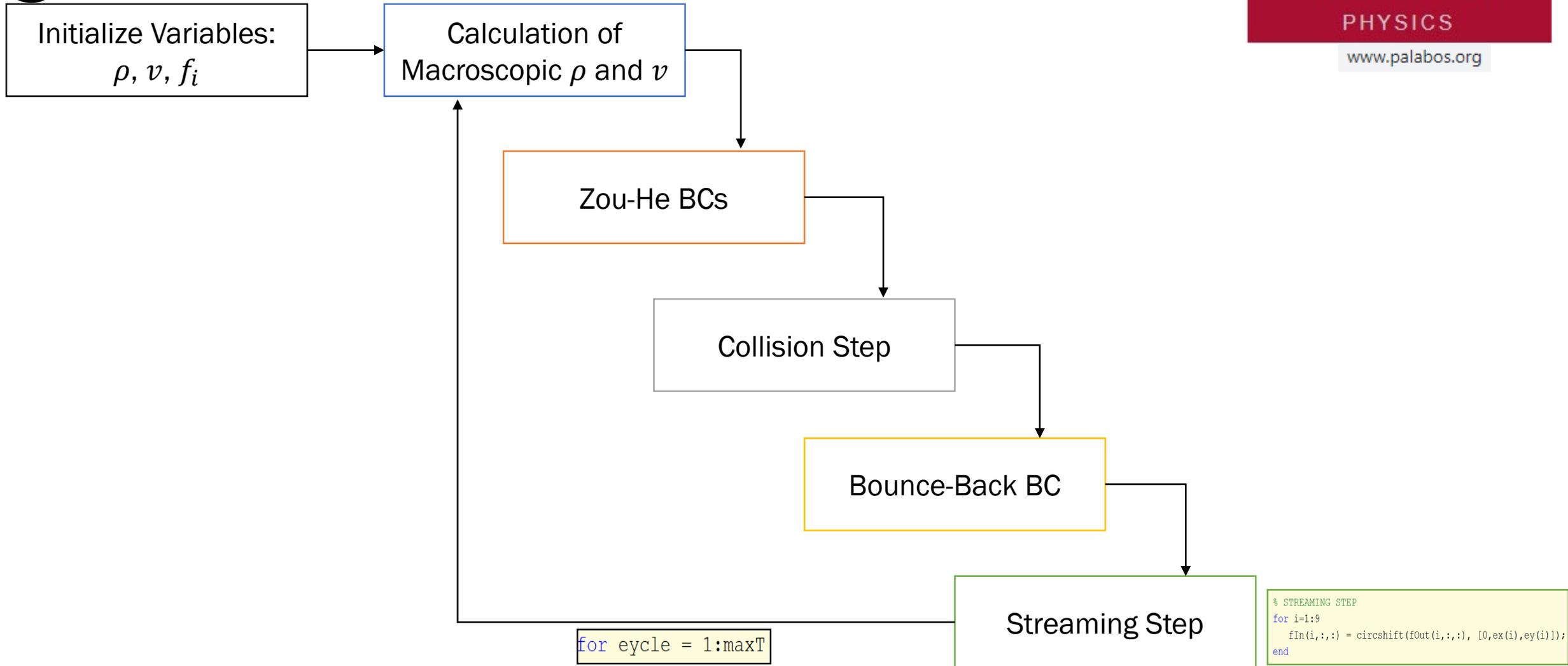
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Numerical Example: Code for Problem Formulation



6

Numerical Example: Code for Problem Formulation



6

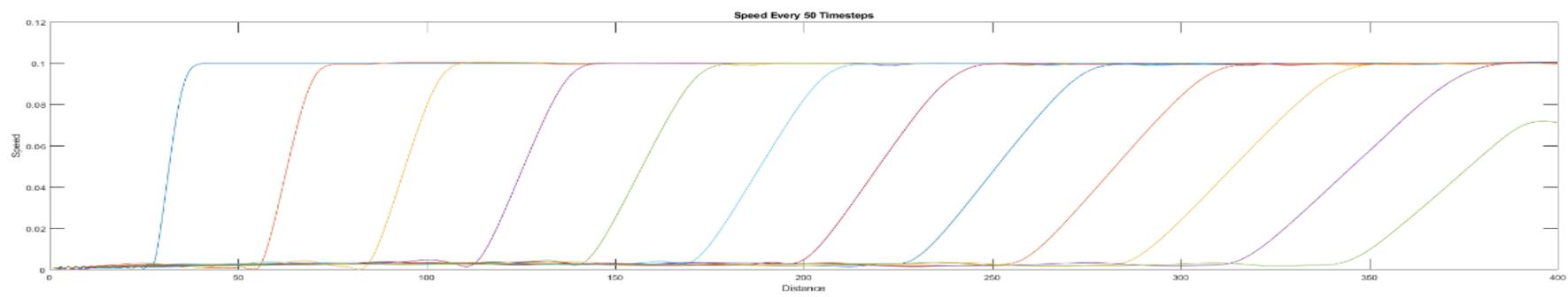
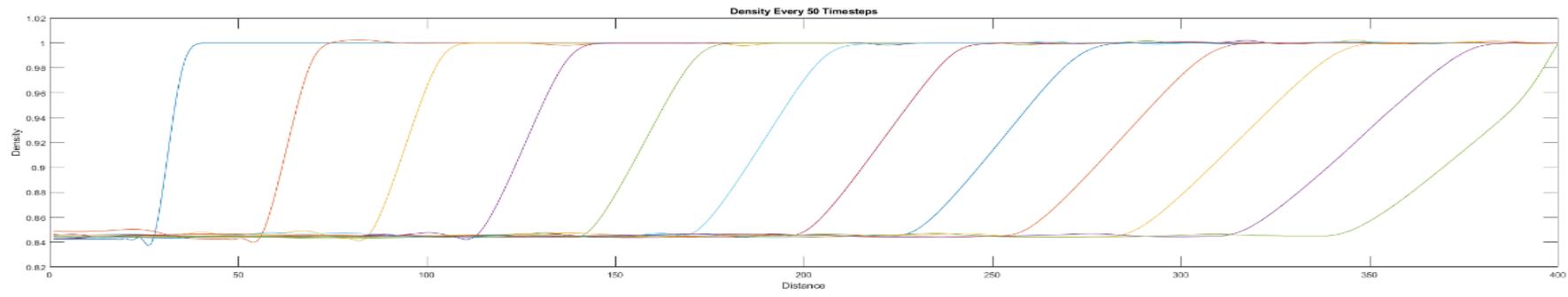
Numeric Example: Case 1 Results

ICs:
 $v_x = 0.1$
 $v_y = 0$
 $\rho = 1$

Zou-He BCs:
 $v_x = 0.001$
 $v_y = 0$
 $\rho = ?$

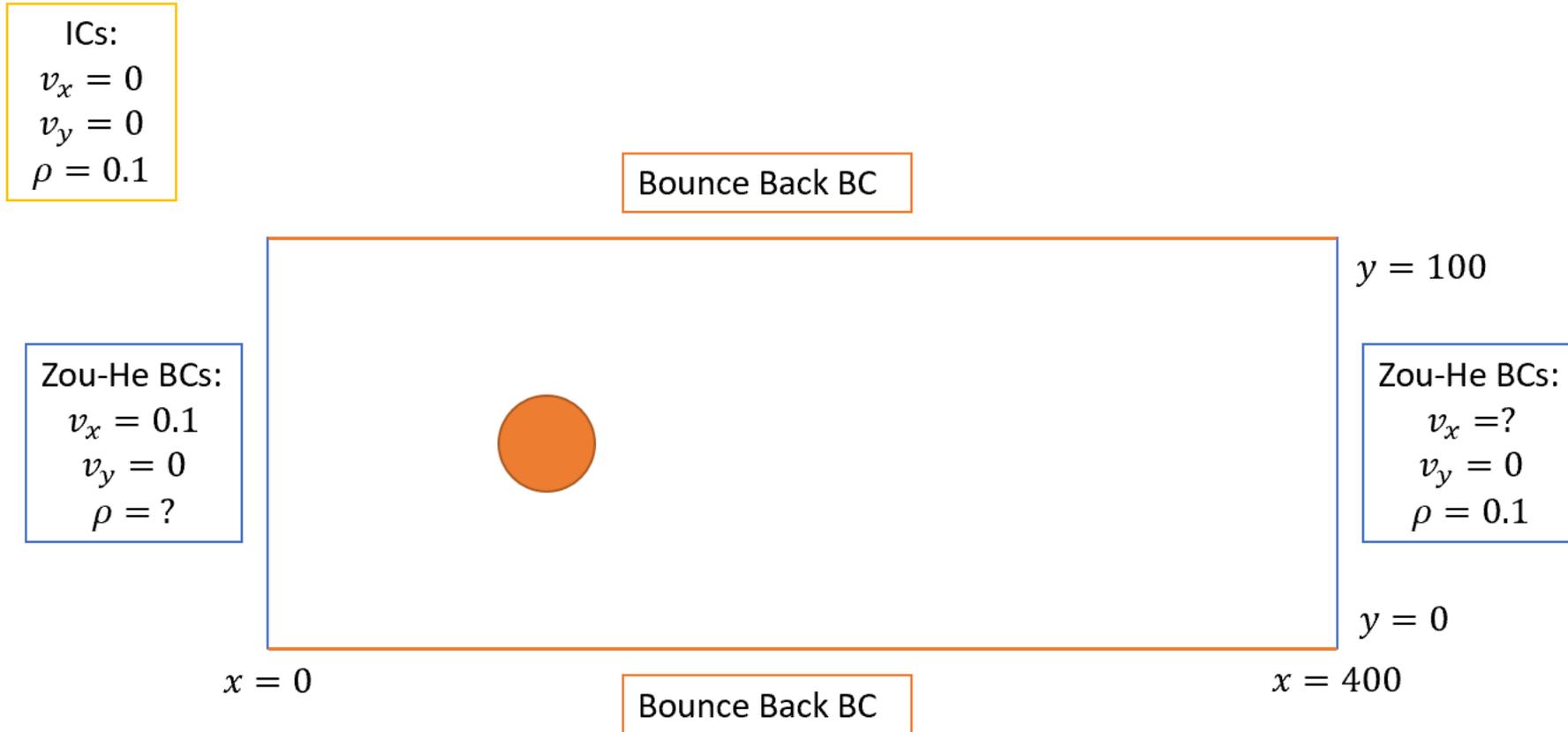


Zou-He BCs:
 $v_x = ?$
 $v_y = 0$
 $\rho = 1$



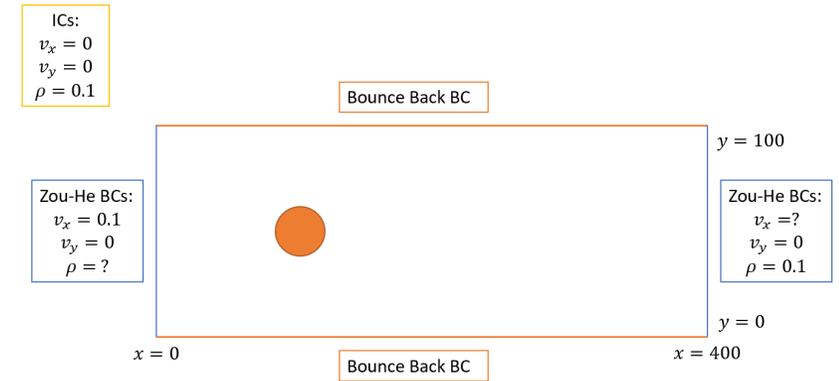
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Numeric Example: Case 2: – Prescribed Rate (Inlet), Prescribed Density (Outlet), Bounce-back Cylinder



6

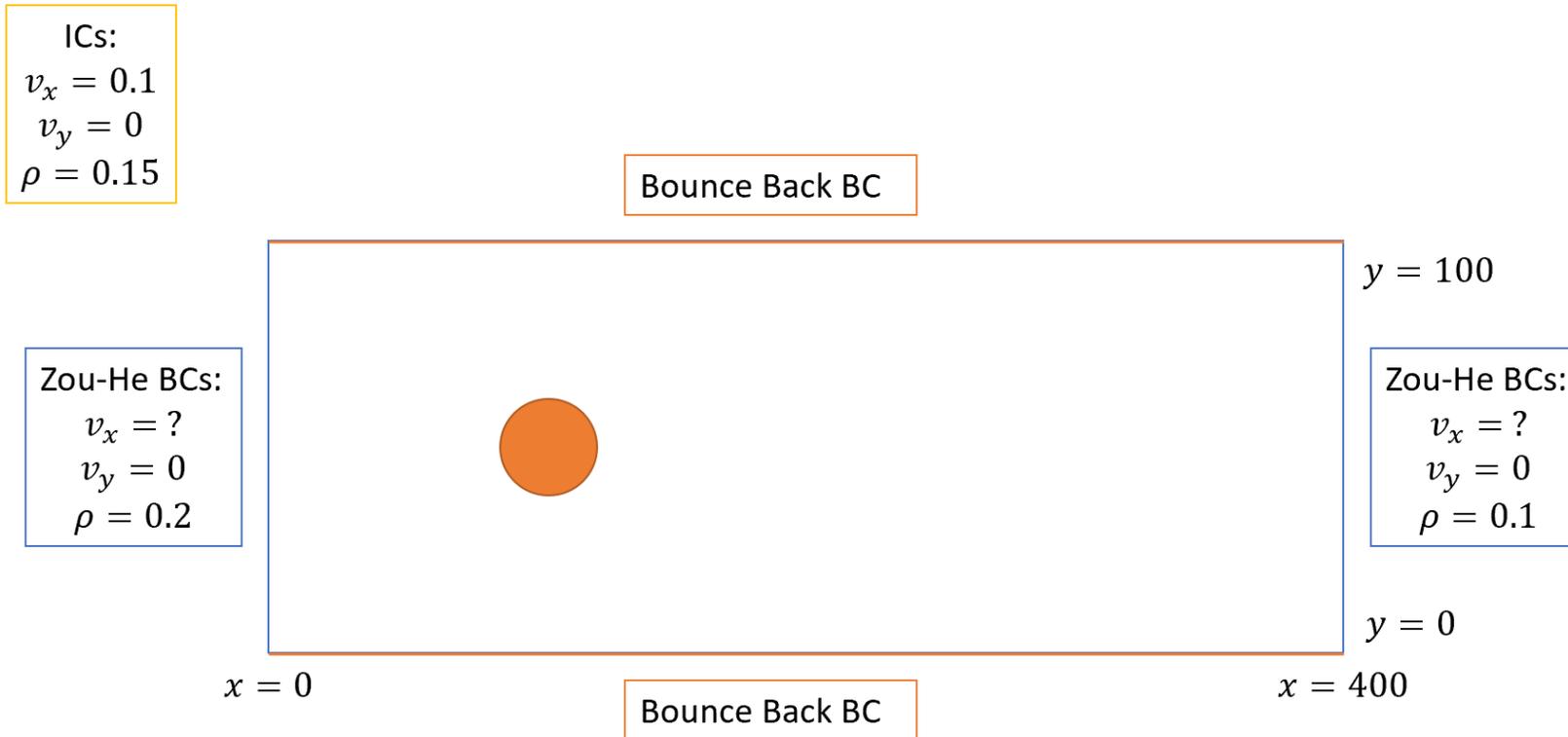
Numeric Example: Case 2 Results



The time-dependent Lattice Boltzmann Method is inefficient for solving steady-state problems, because its speed of convergence is dictated by acoustic propagation, which is very slow

6

Numeric Example: Case 3: – Prescribed Density (Inlet), Prescribed Density (Outlet), BB Cylinder



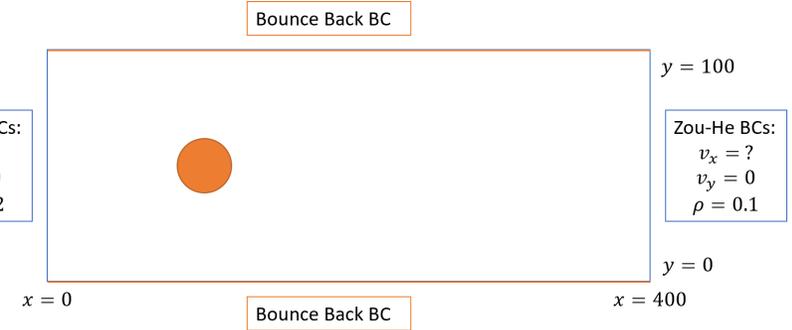
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Numeric Example: Case 3 Results



ICs:
 $v_x = 0.1$
 $v_y = 0$
 $\rho = 0.15$

Zou-He BCs:
 $v_x = ?$
 $v_y = 0$
 $\rho = 0.2$



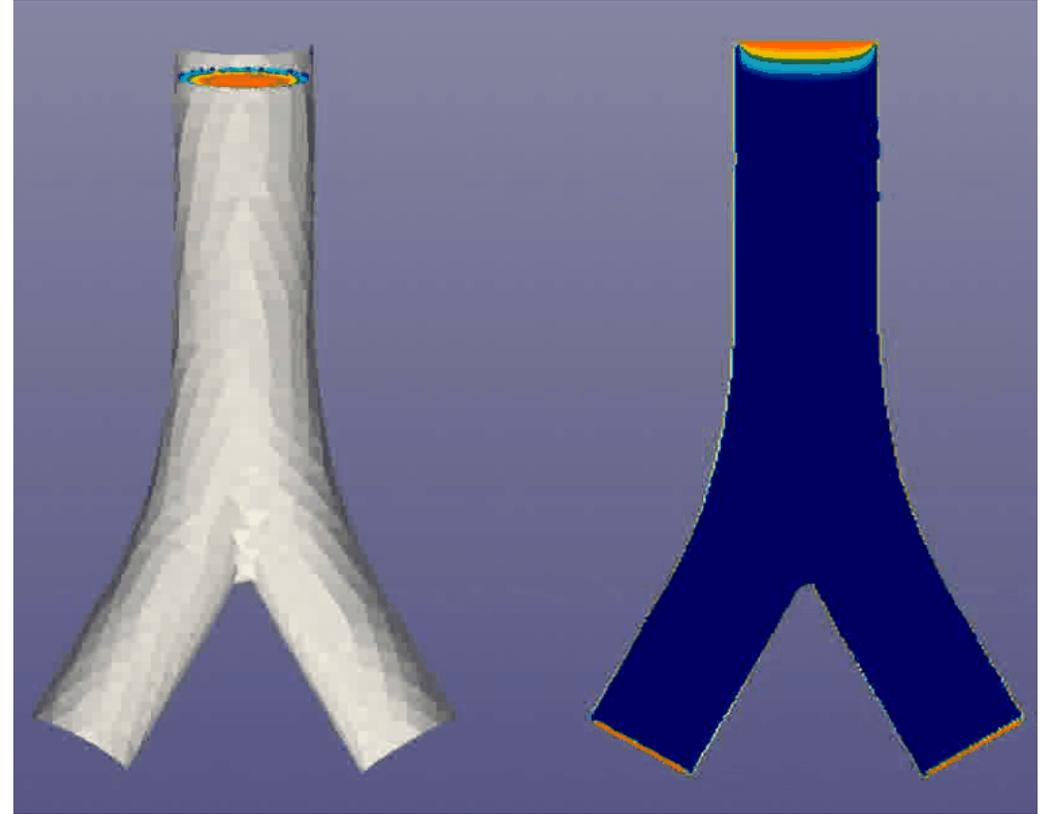
Solution is unstable! Why?

- Largest pressure changes supported are of the order $\frac{\delta P}{P} \sim Ma^2$
- Density difference too large – gives resultant v_x such that Mach number > 0.2
- Solution: model with smaller density change OR model as an external force:

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \boxed{\frac{F}{m} \cdot \frac{\partial f}{\partial v}} = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

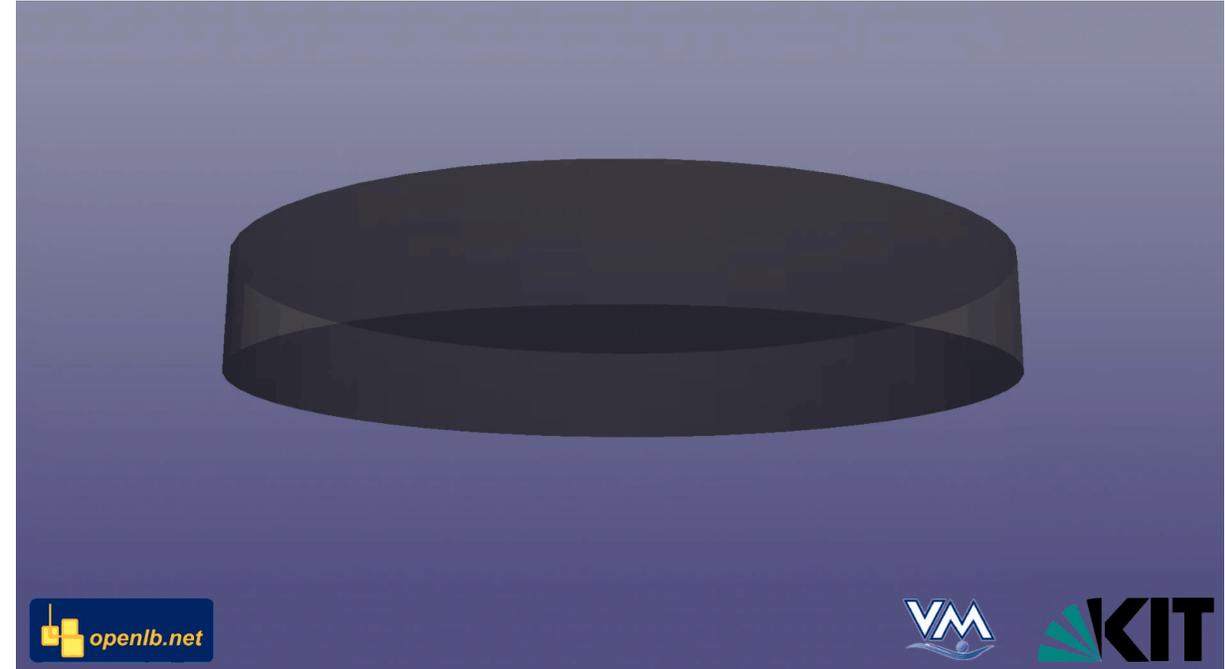
7 Example Applications: Bifurcated Flow in Human Lungs

- Particle flow in human lung important in treatment of asthma and lung cancer
- Important to know where particles deposit depending on their size



7 Example Applications: Cross Flow in Filtration Processes

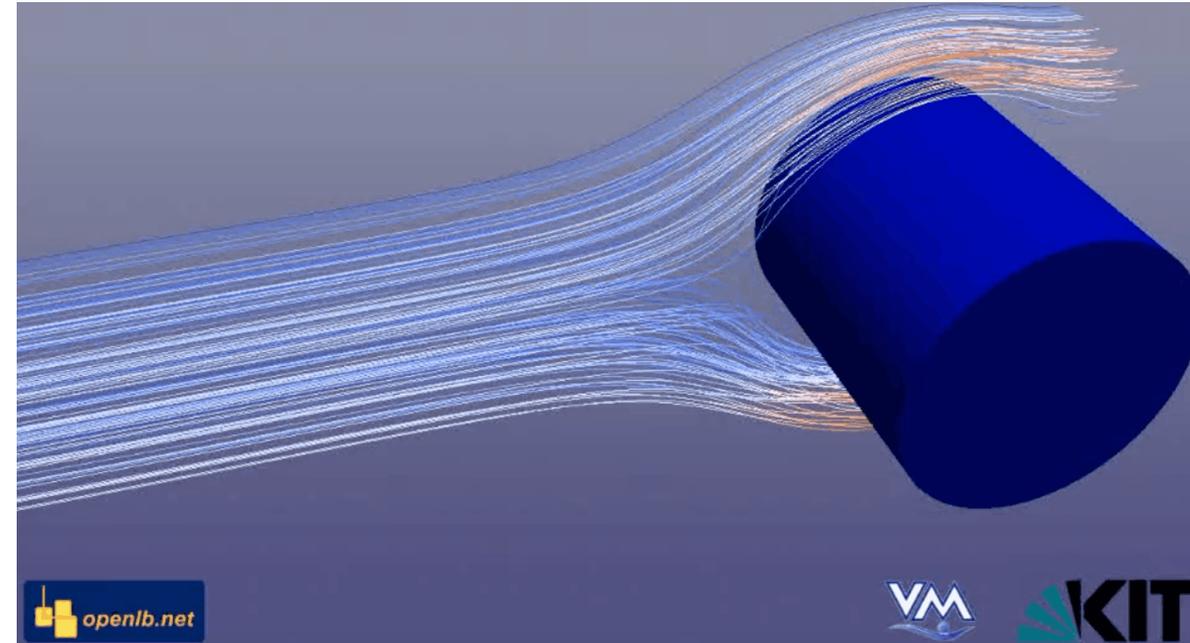
- In filtration processes, performance diminishes over time due to particles blocking the membrane and forming a filter cake
- Flow tangential to the membrane is induced to avoid this process and increase filtration efficiency
- Induced flow prevents deposition, but exposes particles to large shear forces that may destroy them



7

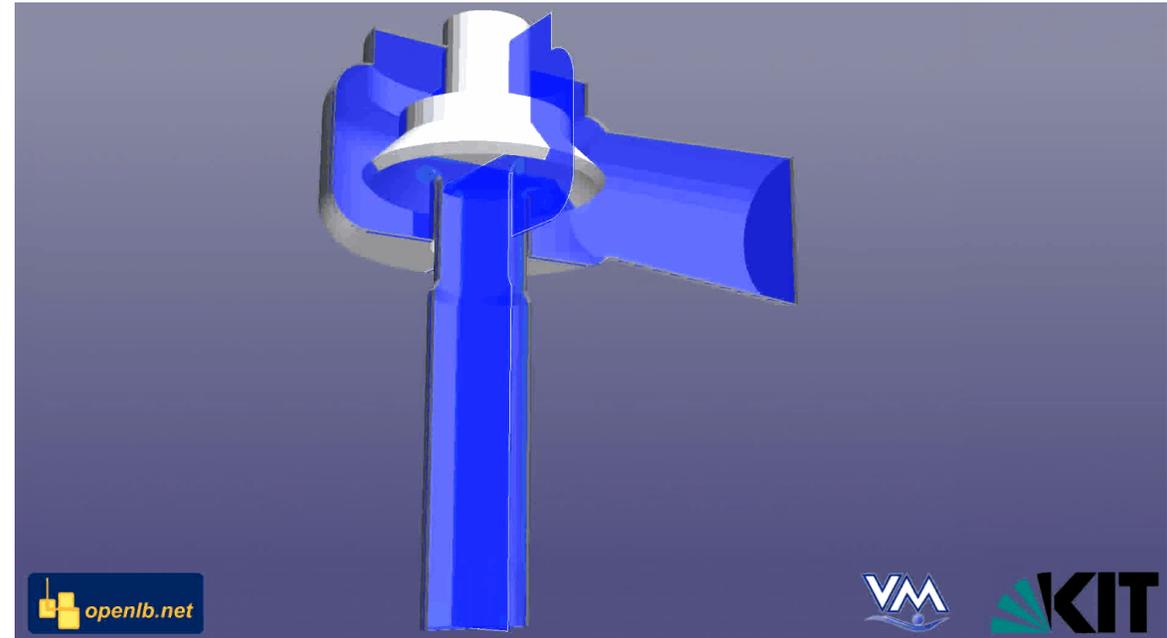
Example Applications: Magnetic Separation

- **High-gradient magnetic fishing (HGMF) can be used for downstream processing of proteins**
- **Magnetic particles are coated with a layer that contains specific ligands for a certain target molecule**
- **The particles are then introduced into a medium containing the target molecule and these molecules adsorb to the ligands**
- **The particles are then separated on a magnetized wire and transferred to another medium**
- **Coupled DEM-LBM approach**



7 Example Applications: Fluid Flow Through a Safety Valve

- Chattering can occur when bleeding off pressure, causing the valve disc to oscillate up and down at a high frequency, reducing pressure dissipation capability and possibly destroying the valve
- Model flow to determine what types of flow cause chatter
- Parallelized LBM to handle unsteady flow



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