Simulation and modeling of natural processes

Week 5: Lattice Boltzmann modeling of fluid flow

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Week 5: Overview

- This week: computer simulation of fluid flow.
- Extension of discrete Cellular Automata to continuum lattice Boltzmann models.
- Part 1: General theory of fluid dynamics.
- Part 2: Write a Python program to simulate fluid flow with the Lattice Boltzmann method.

Computational Fluid Dynamics: Overview

What's a fluid?

A fluid ...

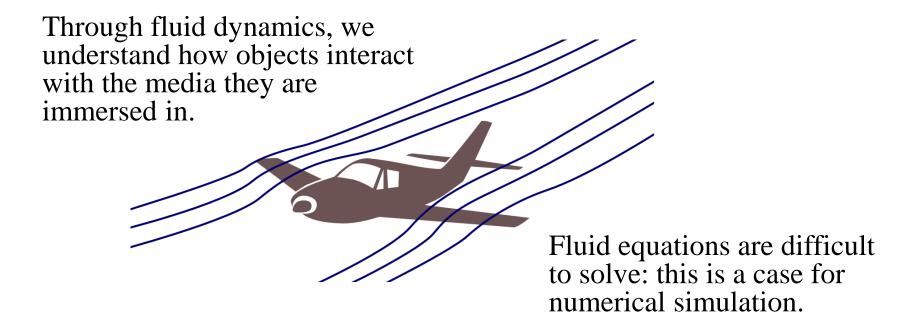
- ... is a substance that continually deforms under stresses.
- ... resists deformations only lightly, because of viscosity.
- ... can adopt the shape of any container into which it flows.

Fluids include:

- Liquids
- Gases
- Plasmas

Fluid = Continuum Model

Why fluid dynamics?



Fluid dynamics is everywhere

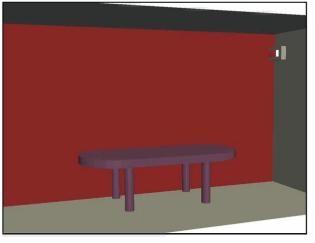
Important application areas are found

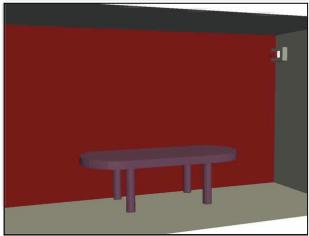
- In physics.
- In biology and medical physics.
- In chemistry.
- In geology.
- ... and many more.

Example 1: Heat convection

Air-conditioner in a meeting room







Fixed air-conditioner

Sweeping air-conditioner

Example 2: Blood flow in an artery

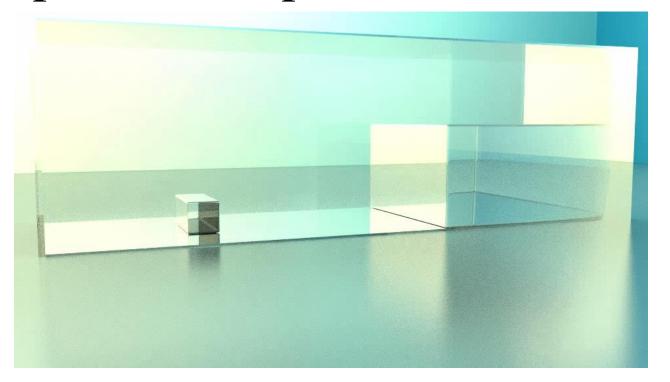


Segment of a human artery with an aneurysm (balloon-like bulge).

Simulation:

- Fluid dynamics of pulsatile blood flow.
- Embedded red blood cells.
- Blood clotting inside aneurysm, with change of geometry.

Example 3: Collapse of a water column



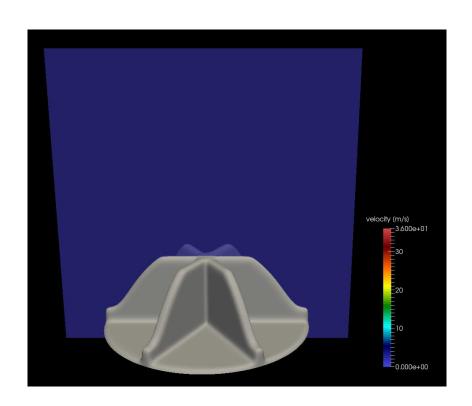
Example 4: washing machine



Simulation:

- Water fluid flow.
- Rotating agitator.
- Embedded flexible tissue, 2-way coupled with the water.

Example 4: washing machine



Washing machine: velocity field.

Credits

I'd like to thank

- Orestis Malaspinas (University of Geneva) for the blood flow example.
- **Dimitrios Kontaxakis** (FlowKit Ltd, Lausanne) for the example of a washing machine.
- Andrea Parmigiani (University of Geneva) and Andrea Di Blasio (FlowKit Ltd, Lausanne) for water column example.

End of module Computational Fluid Dynamics: Overview

Coming next

Computational Fluid Dynamics: Equations and challenges

Computational Fluid Dynamics: Equations and challenges

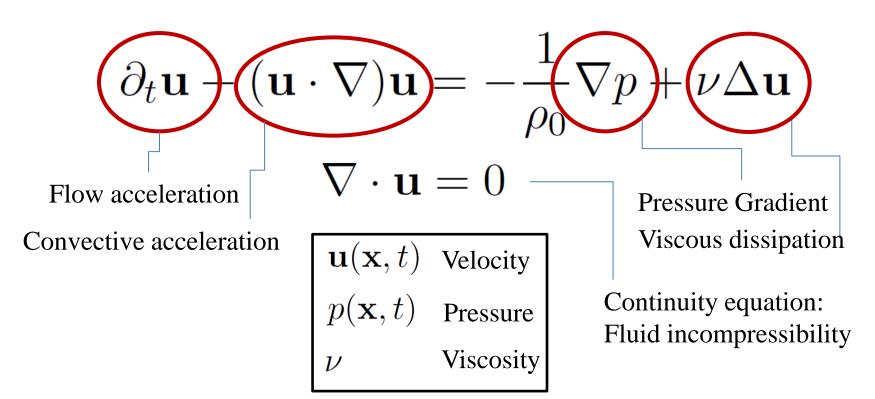
The Navier-Stokes equations

The basis: Navier-Stokes equations for incompressible flow. They don't account for

- Fluid compressibility in gases.
- Thermal effects.
- Chemical reactions.
- ... many more.

And yet, they are very frequently and successfully used, for both liquids and gases.

The Navier-Stokes equations



Dimensionless formulation

Choose a...

Characteristic velocity: U

Characteristic length: L

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho_0} \nabla p + \nu \Delta \mathbf{u}$$

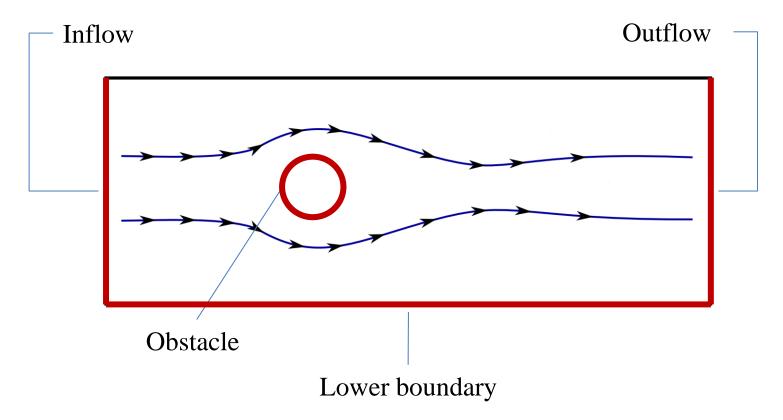
$$\vec{u}^* = \frac{\vec{u}}{U}$$
 $\partial_t^* = \frac{L}{U}\partial_t$ $p^* = \frac{p}{\rho_0 U^2}$ $\vec{\nabla}^* = L\vec{\nabla}$

Reynolds number:

$$Re = \frac{UL}{\nu}$$

$$\partial_t^* \mathbf{u}^* + (\mathbf{u}^* \cdot \nabla^*) \mathbf{u}^* = -\nabla p^* + \frac{\nu}{UL} \Delta \mathbf{u}^*$$

Boundary Conditions



End of module

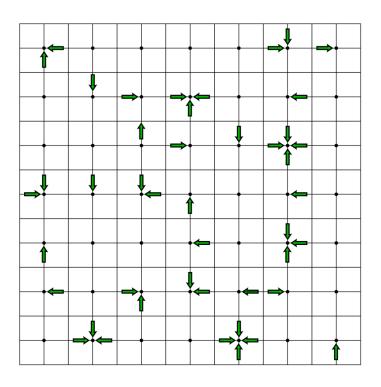
Computational Fluid Dynamics: Equations and challenges

Coming next

From Lattice Gas to Lattice Boltzmann

From Lattice Gas to Lattice Boltzmann

Lattice Gas Automata: Reminder



The lattice gas automaton HPP

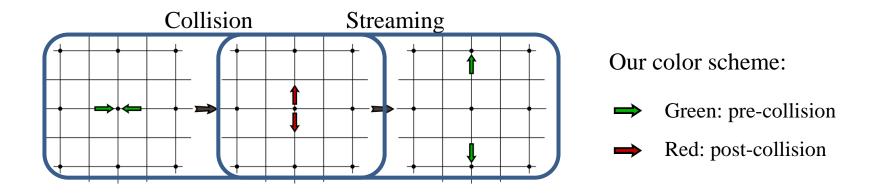
- Discrete Boolean states.
- Each cell is populated by four particles at most.
- Each of the four storage locations corresponds to a direction of propagation of the particle.

Comment

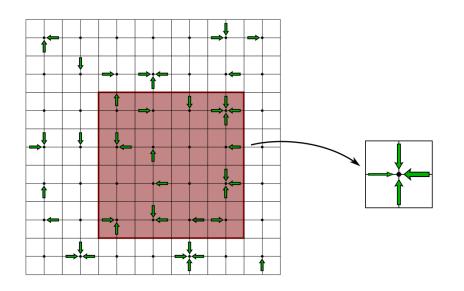
 This mesoscopic model describes the dynamics of a gas, not a liquid.

Lattice Gas Automata: Reminder

- When several particles meet on a node, they collide: all physics takes place here.
- After collision, particles are streamed to a nearest neighbor.



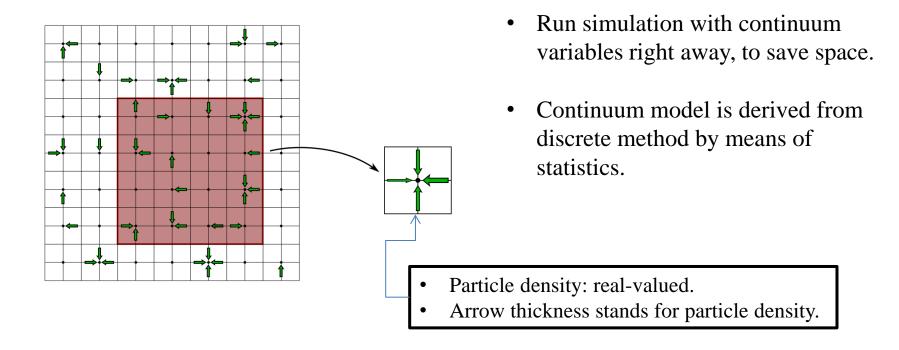
From discrete to continuum variables



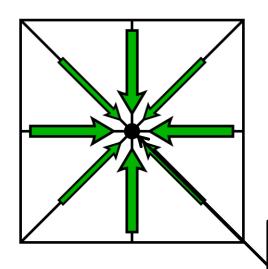
In a lattice gas automaton:

- Run the simulation with discrete variables.
- At the end, extract macroscopic variables by taking averages.

Lattice Boltzmann Method: Idea



Lattice Boltzmann Method: details

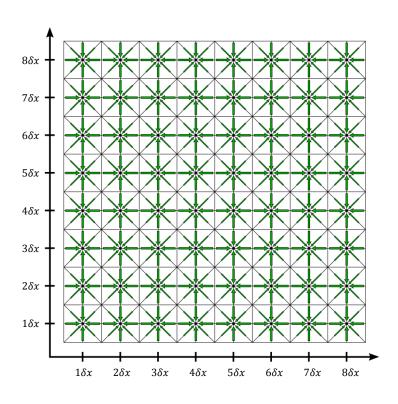


Lattice Boltzmann 2D model D2Q9:

- Four directions aren't quite enough.
- Nine directions: eight connections to nearest neighbors + «rest population».
- Variables representing particle densities are called «populations».

«Rest population» particles stay on a cell, don't travel to neighbors during streaming.

Lattice Boltzmann Variables



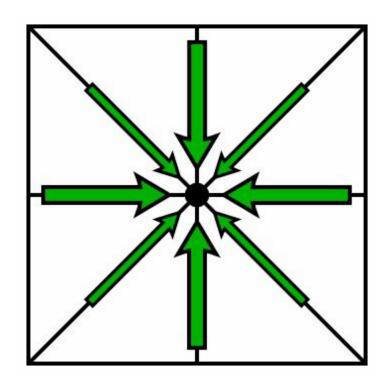
Space Discretization:

- Every cell represents flow variables at a point in space.
- Equal distance δx between cells in x- and y-direction.
- To represent space with 8x8 points, we need a total of 8x8x9 = 576 floating point variables.

Python code to allocate memory:

$$f = zeros(9, 8, 8)$$

Collision step



- Like in lattice gas: collision maps pre-collision populations to postcollision populations.
- All populations are modified during collision. Changes are not visible on video, because they are small perturbations.

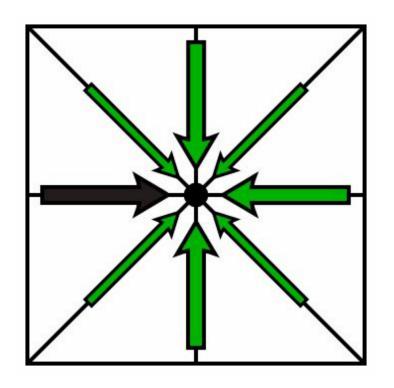
Our color scheme:



Green: pre-collision

Red: post-collision

Collision step



Model:

- Collision is instantaneous.
- Collision is localized at cell coordinates.

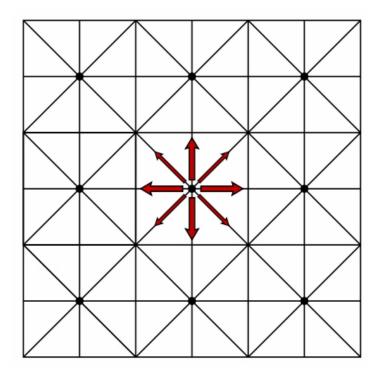
Our color scheme:



Green: pre-collision

Red: post-collision

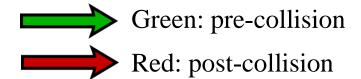
Streaming step



Model:

- Streaming takes the system from time t to time $t + \delta t$.
- Streaming includes nearestneighbor access.

Our color scheme:



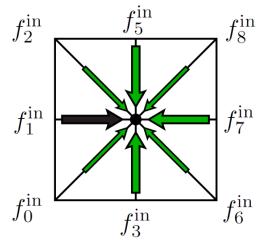
End of module From Lattice Gas to Lattice Boltzmann

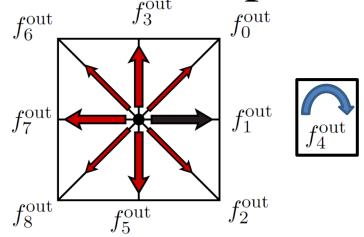
Coming next Macroscopic Variables

Macroscopic Variables

Back to the collision step







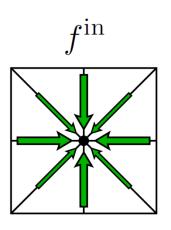
Pre-collision: $f_i^{\text{in}}(\mathbf{x}, t)$ «Incoming populations»

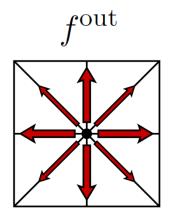
Post-collision: $f_i^{\mathrm{out}}(\mathbf{x},t)$ «Outgoing populations»

The index *i* runs from 0 to 8.

Pre- and post-collision: variables

In our Python code, we save incoming and outgoing populations in separate matrices.





Python code:

```
# assign some size
nx, ny = ...
fin = zeros(9, nx, ny)
fout = zeros(9, nx, ny)
```

Density

Particle density is defined the same as in a lattice gas automaton:

$$\rho(\boldsymbol{x},t) = \sum_{i=0}^{8} f_i^{\text{in}}(\boldsymbol{x},t)$$

Each cell has its own density, which is the sum of the nine populations.

Density

$$\rho(\boldsymbol{x},t) = \sum_{i=0}^{8} f_i^{\text{in}}(\boldsymbol{x},t)$$

Python code:

```
rho = zeros((nx, ny))
for ix in range(nx):
    for iy in range(ny):
        rho[ix, iy] = 0
        for i in range(9):
        rho[ix,iy] += fin[i, ix, iy]
```

Simpler and faster, with NumPy array-based syntax:

Pressure

Pressure is proportional to density, according to the ideal gas law, at constant temperature:

$$p = c_s^2 \rho$$

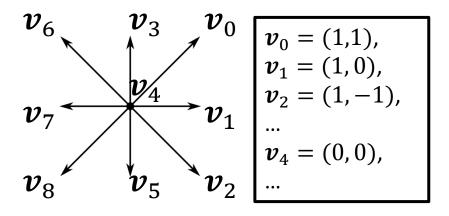
The speed of sound c_s is, in our D2Q9 model, a lattice constant:

$$c_s^2 = \frac{1}{3} \frac{\delta x^2}{\delta t^2}$$

Units: Say that δx has units of meters [m] and δt has units of seconds [s]. Then pressure has units of $\frac{m^2}{s^2}$. Multiply this by the physical density of our fluid $(e. g. 1 \frac{kg}{m^3})$ to obtain units of Pascal $(\frac{kg}{ms^2})$.

Velocity

Let's introduce a set of 9 vectors:



They are called lattice velocities: If there's a cell at position x, there's also one at $x + v_i \delta t$.

Again, velocity is defined just the same as in a lattice gas automaton:

$$\boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{\rho(\boldsymbol{x},t)} \frac{\delta x}{\delta t} \sum_{i=0}^{8} \boldsymbol{v}_i f_i^{\text{in}}(\boldsymbol{x},t)$$

Velocity

```
v = array([[1, 1], [1, 0], [1, -1], [0, 1], [0, 0], [0, -1], [-1, 1], [-1, 0], [-1, -1]])
```

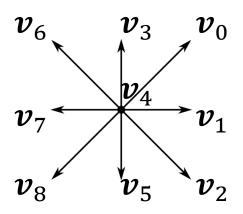
Traditional Python code:

```
u = zeros((2, nx, ny))
for ix in range(nx):
  for iy in range(ny):
     u[0, ix, iy] = 0
     u[1, ix, iy] = 0
     for i in range(9):
         u[0, ix, iy] += v[i, 0] * fin[i, ix, iy]
        u[1, ix, iy] += v[i,1] * fin[i, ix, iy]
     u[0, ix, iy] /= rho[ix, iy]
     u[1, ix, iy] /= rho[ix, iy]
```

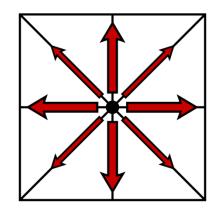
Simpler and faster, with NumPy array-based syntax:

```
u = zeros((2, nx, ny))
for i in range(9):
    u[0,:,:] += v[i,0] * fin[i,:,:]
    u[1,:,:] += v[i,1] * fin[i,:,:]
u /= rho
```

Don't be confused



- These are 9 2D vectors.
- They have constant values.



- These are 9 scalar values.
- Their value is time-dependent.

End of module Macroscopic variables

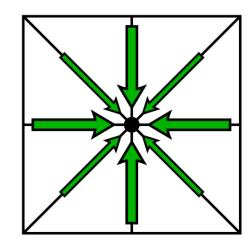
Coming next

Collision step: the BGK model

Collision step: the BGK model

What's the value of the populations?

- So far, we have interpreted populations as particle averages of a lattice gas automaton.
- Alternative interpretation: populations are probability densities of particles in a real gas.
- In kinetic theory, gas densities are described by a single probability density function f(x, v, t).
- The motion of f is described by the *Boltzmann* equation.

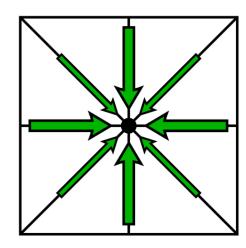


What's the value of the populations?

- When a gas is macroscopically at rest, or has a constant velocity **u**, its molecules are still moving.
- The distribution of their velocities v at every point x in space is given by a *Maxwell-Boltzmann distribution*:

$$f(\mathbf{x}, \mathbf{v}, t) \sim e^{|\mathbf{v} - \mathbf{u}|^2}$$
.

• Even when it moves, a gas remains close to its equilibrium state. We consider its motion as a *perturbation around the equilibrium*.



Collision: BGK model

Inspired by kinetic theory, we formulate the collision term in lattice Boltzmann as a relaxation to local equilibrium:

$$f_i^{\text{out}} - f_i^{\text{in}} = -\omega \left(f_i^{\text{in}} - E(i, \rho, \vec{u}) \right)$$

- E is the local equilibrium. It depends on the macroscopic variables and has a different value for every direction i.
- The parameter ω is the frequency of relaxation.
- This collision model is called the *BGK model*.

Collision frequency and viscosity

- If ω is small, the fluid converges only slowly to its equilibrium: it is highly viscous.
- More generally, on can show that the fluid viscosity depends inversely on the relaxation parameter ω :

$$\nu = \delta t \, c_s^2 \left(\frac{1}{\omega} - \frac{1}{2} \right)$$

Collision: BGK model

The equilibrium is obtained as a truncated series of the Maxwell-Boltzmann distribution:

$$E(i, \rho, \boldsymbol{u}) = \rho t_i \left(1 + \frac{\boldsymbol{v_i} \cdot \boldsymbol{u}}{c_s^2} + \frac{1}{2 c_s^4} (\boldsymbol{v_i} \cdot \boldsymbol{u})^2 - \frac{1}{2 c_s^2} |\boldsymbol{u}|^2 \right)$$

- The constants t_i compensate for the different lengths of velocities v_i .
- t_i is 1/9 for orthogonal directions, 1/36 for diagonal directions, and 4/9 for the rest velocity:

t = array([1/36, 1/9, 1/36, 1/9, 4/9, 1/9, 1/36, 1/9, 1/36])

Collision: Python codes

Equilibrium:

We write the code in «lattice units», i.e. with $\delta x = \delta t = 1$.

$$E(i, \rho, \boldsymbol{u}) = \rho t_i \left(1 + \frac{\boldsymbol{v_i} \cdot \boldsymbol{u}}{c_s^2} + \frac{1}{2 c_s^4} (\boldsymbol{v_i} \cdot \boldsymbol{u})^2 - \frac{1}{2 c_s^2} |\boldsymbol{u}|^2 \right)$$

```
def equilibrium(rho, u):

usqr = 3/2 * (u[0]**2 + u[1]**2)

eq = zeros((9, nx, ny))

for i in range(9):

vu = 3 * (v[i,0]*u[0,:,:] + v[i,1]*u[1,:,:])

eq[i,:,:] = rho*t[i] * (1 + vu + 0.5*vu**2 - usqr)

return eq
```

Collision: Python codes

Collision:

$$f_i^{\text{out}} - f_i^{\text{in}} = -\omega \left(f_i^{\text{in}} - E(i, \rho, \vec{u}) \right)$$

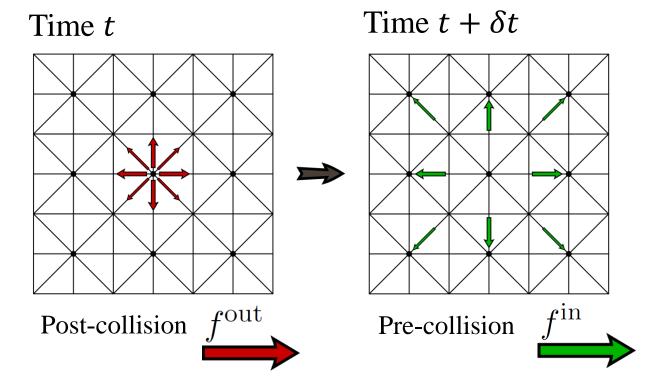
End of module Collision step: the BGK model

Coming next
Streaming Step

The streaming step

Streaming step

Streaming takes the system to the next time iteration, $t + \delta t$



Streaming step: code

Conventional Python code:

- On boundaries, we apply periodicity.
- If a population leaves the domain, it enters the domain again on the other side.

```
for ix in range(nx):
  for iy in range(ny):
     for i in range(9):
        next x = ix + v[i,0]
        if next x < 0: next_x = nx-1
        if next x >= nx: next x = 0
        next y = iy + v[i,1]
        if next x < 0: next x = nx-1
        if next x >= nx: next x = 0
       fin[i, next_x,next_y] = fout[i, ix, iy]
```

Streaming step: code

Conventional Python code:

```
for ix in range(nx):
    for iy in range(ny):
        for i in range(9):
            next_x = ix + v[i,0]
            if next_x < 0: next_x = nx-1
            if next_x >= nx: next_x = 0

            next_y = iy + v[i,1]
            if next_x < 0: next_x = nx-1
            if next_x >= nx: next_x = 0
            fin[i, next_x, next_y] = fout[i, ix, iy]
```

NumPy Array-based code:

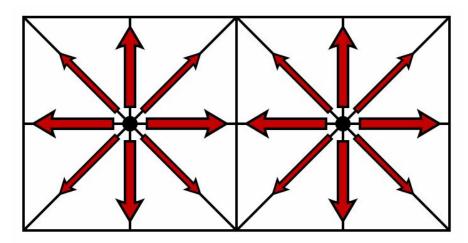
```
for i in range(9):
    fin[i,:,:] = roll(
        roll(fout[i,:,:], v[i,0], axis=0),
        v[i,1], axis=1)
```

Do we really need double the memory?

- So far we allocated two sets of populations f^{in} and f^{out} .
- Could we spare one, and store both pre-collision and post-collision in the same variable *f*?
- Answer: yes, but it needs some care.
- I will show how to do it. But for simplicity, we keep our code with two sets of populations.

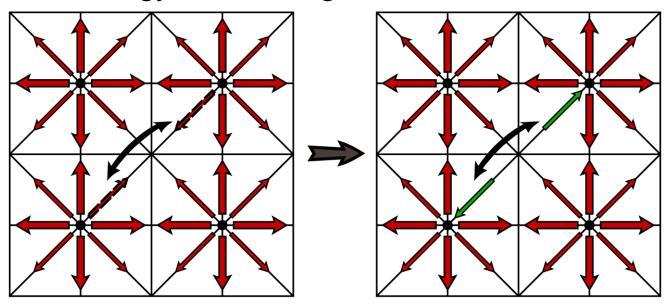
Single-population implementation

- Collision step, no problem: it is local. Simply overwrite f^{in} with f^{out} .
- Streaming step, more tricky. As you stream populations to a neighbor, you risk overwriting one that is still needed.
- Solution: *stream to the neighbor* and *from the neighbor* at the same time, exchanging populations instead of overwriting them.



Single-population implementation

This strategy works along all directions:

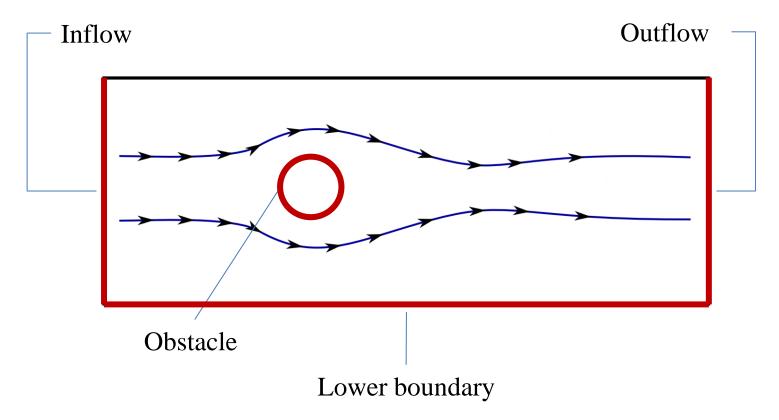


End of module Streaming Step

Coming next
Boundary conditions

Boundary conditions

Boundary conditions



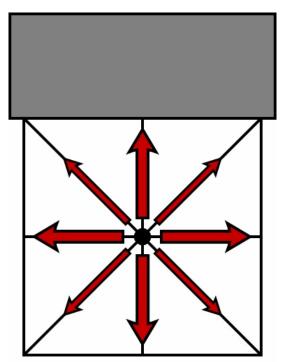
Boundary conditions

- We need different types of boundary conditions:
 - Inflow: imposes the velocity profile.
 - Outflow, and lower and upper boundary: pretend that the domain is larger.
 - Physical obstacle.
- There exists already a boundary condition in our code: periodicity.
 - Behaves as if our simulation was repeated an infinitely many times.
 - We will use periodicity for lower/upper boundary.

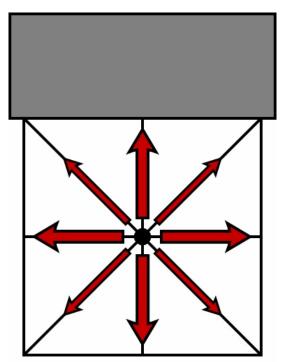
Obstacle: no-slip wall

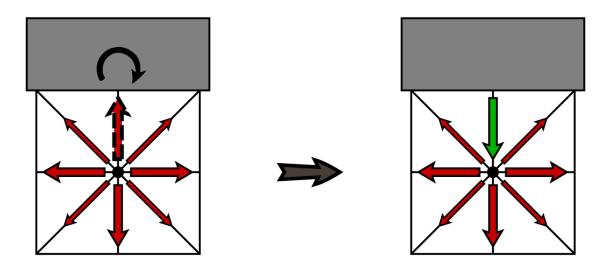
- Most physical obstacles act like no-slip walls.
- Macroscopically: the velocity is zero along the wall.
- At the molecular level: the obstacle has a surface roughness, and molecules «adhere» to the surface.
- Not all obstacles have a no-slip condition. Example: an air bubble in water is smooth, even at molecular level.

- The bounce-back condition is a way to implement a no-slip wall in lattice Boltzmann.
- During streaming, a population which leaves the fluid and hits an obstacle «bounces back».
- Its value is unchanged, and it is copied to the population with reverse direction.

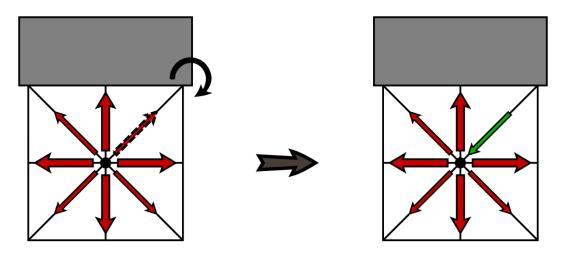


- The bounce-back condition is a way to implement a no-slip wall in lattice Boltzmann.
- During streaming, a population which leaves the fluid and hits an obstacle «bounces back».
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This condition mimicks the physical process that occurs when molecules hit a wall.

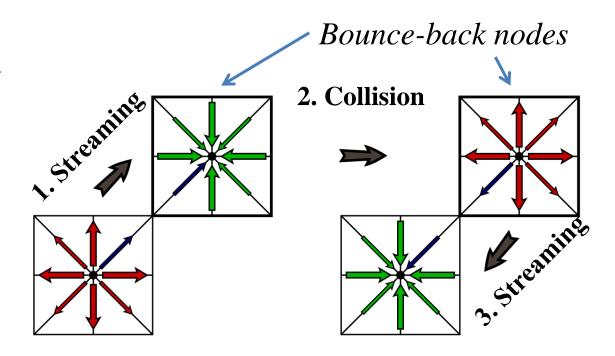


- Attention: populations on diagonal directions are not reflected like on a mirror. They also bounce-back to where they came from.
- This reflects the fact that at a molecular level, the obstacle is rough, and not smooth like a mirror.

- Bounce-back is simple: track all populations that hit an obstacle, and send them back.
- Yet, this involves quite some book-keeping. Which nodes are affected? Which directions?
- Simpler solution: let the populations travel into the obstacle. Then, we revert them inside the obstacle, and send them back.
- No bookkeeping of directions. All cells inside an obstacle are bounce-back cells: instead of colliding, they revert all the directions.

The bounce-back cycle

During collision, a bounce-back node replaces every population by the one in the opposite direction.



The bounce-back cycle

Instead of colliding, bounce-back nodes implement the following relation:

$$f_i^{\text{in}}(\boldsymbol{x}, t+1) = f_j^{\text{out}}(\boldsymbol{x}, t)$$

where direction *i* is opposite to direction *j*:

$$|v_i = -v_j|$$

Bounce-back: code

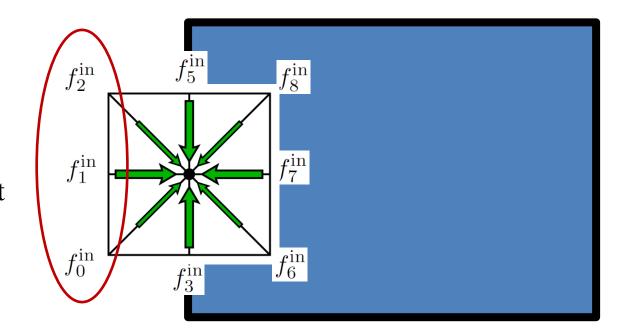
NumPy array-based code:

```
for i in range(9):
    fout[i, obstacle] = fin[8-i, obstacle]
```

We have on purpose listed the lattice velocities in such a way that the direction opposite to i is given by 8-i.

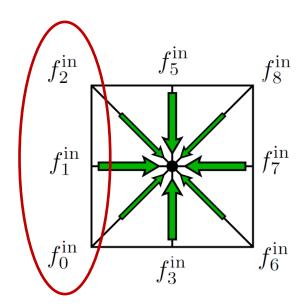
Inflow condition

After streaming, the populations f_0 , f_1 , and f_2 are unknown on all cells along the left boundary.



Inflow condition

- We want to impose a velocity \boldsymbol{u} on inflow boundary cells. So, \boldsymbol{u} is known. But what about ρ ? And what about f_0 , f_1 , and f_2 ?
- We must extract this missing information using the known populations, and using u.



Inflow condition: density

Remember:

$$\rho(\boldsymbol{x},t) = \sum_{i=0}^{8} f_i^{\text{in}}(\boldsymbol{x},t)$$

$$\rho(\boldsymbol{x},t) = \sum_{i=0}^{8} f_i^{\text{in}}(\boldsymbol{x},t) \left| \boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{\rho(\boldsymbol{x},t)} \frac{\delta x}{\delta t} \sum_{i=0}^{8} \boldsymbol{v}_i f_i^{\text{in}}(\boldsymbol{x},t) \right|$$

Let's define:

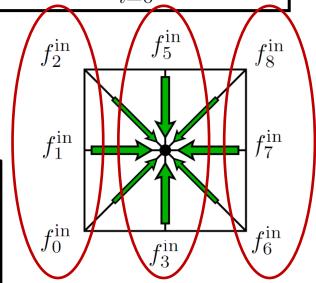
- $\rho_1 = f_0 + f_1 + f_2$ (unknown)
- $\rho_2 = f_3 + f_4 + f_5$ (known)
- $\rho_3 = f_6 + f_7 + f_8$ (known)

Then:

- $\rho = \rho_1 + \rho_2 + \rho_3$
- $\rho u_x = \rho_1 \rho_3$

And hence:

$$\rho = \frac{\rho_2 + 2\rho_3}{1 - u_x}$$



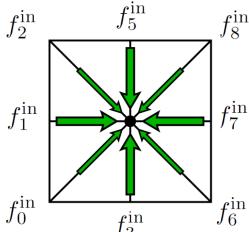
Inflow condition: unknown populations

- Remember: populations are always close to their equilibrium.
- We first initialize the unknown populations to their equilibrium value.
- Then, we check how much the opposite population deviates from equilibrium, at add this value as a correction.

$$f_0^{\text{in}} = E(0, \rho, \mathbf{u}) + (f_8^{\text{in}} - E(8, \rho, \mathbf{u}))$$

$$f_1^{\text{in}} = E(1, \rho, \mathbf{u}) + (f_7^{\text{in}} - E(7, \rho, \mathbf{u}))$$

$$f_2^{\text{in}} = E(2, \rho, \mathbf{u}) + (f_6^{\text{in}} - E(6, \rho, \mathbf{u}))$$



Inflow condition: code

Define the indices of the three columns:

```
col1 = array([0, 1, 2])
col2 = array([3, 4, 5])
col3 = array([6, 7, 8])
```

• Calculate the density:

```
rho[0,:] = 1/(1-u[0,0,:]) * ( sum(fin[col2,0,:], axis=0) + 2*sum(fin[col3,0,:], axis=0) )
```

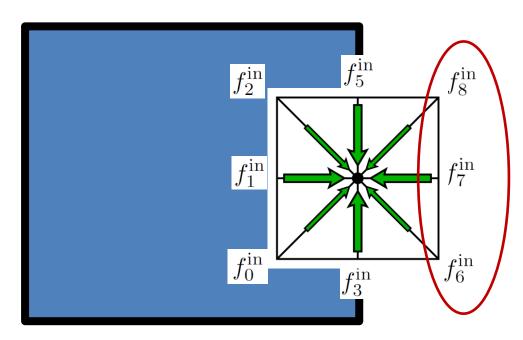
• Calculate the populations:

```
fin[[0,1,2],0,:] = feq[[0,1,2],0,:] + fin[[8,7,6],0,:] - feq[[8,7,6],0,:]
```

Outflow condition

- The outflow boundary must behave as if the domain didn't end.
- For the unknown populations, f_6 , f_7 , and f_8 , we simply copy the value from the neighboring cell, right behind.

fin[col3,-1,:] = fin[col3,-2,:]



End of module Boundary conditions

Coming next

Application: flow around an obstacle

Application: flow around an obstacle

Our code: all pieces put together

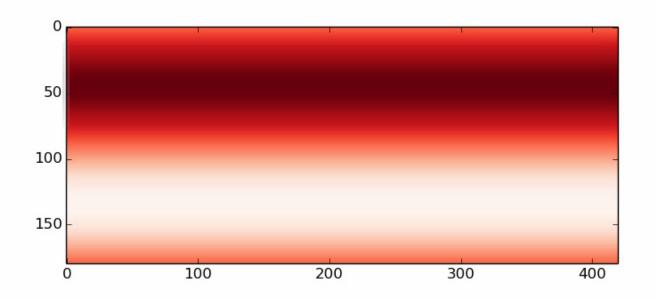
```
#!/usr/bin/pvthon3
# Copyright (C) 2015 Universite de Geneve, Switzerland
# E-mail contact: jonas.latt@unige.ch
# 2D flow around a cylinder
from numpy import *
import matplotlib.pyplot as plt
from matplotlib import cm
maxIter = 200000 # Total number of time iterations.
Re = 10.0
              # Reynolds number.
nx. nv = 420, 180 # Numer of lattice nodes.
              # Height of the domain in lattice units.
cx, cy, r = nx//4, ny//2, ny//9 # Coordinates of the cylinder.
uLB = 0.04
                          # Velocity in lattice units.
nulb = uLB*r/Re;
                          # Viscoscity in lattice units.
omega = 1 / (3*nulb+0.5); # Relaxation parameter.
v = array([[1, 1], [1, 0], [1, -1], [0, 1], [0, 0],
          [ 0, -1], [-1, 1], [-1, 0], [-1, -1] ])
t = array([1/36, 1/9, 1/36, 1/9, 4/9, 1/9, 1/36, 1/9, 1/36])
col1 = array([0, 1, 2])
col2 = array([3, 4, 5])
col3 = array([6, 7, 8])
def macroscopic(fin):
   rho = sum(fin, axis=0)
   u = zeros((2, nx, nv))
   for i in range (9):
      u[0,:,:] += v[i,0] * fin[i,:,:]
      u[1,:,:] += v[i,1] * fin[i,:,:]
   u /= rho
   return rho, u
def equilibrium(rho, u):
                               # Equilibrium distribution function.
   usgr = 3/2 * (u[0]**2 + u[1]**2)
   feg = zeros((9,nx,nv))
   for i in range (9):
      cu = 3 * (v[i,0]*u[0,:,:] + v[i,1]*u[1,:,:])
      feg[i,:,:] = rho*t[i] * (1 + cu + 0.5*cu**2 - usgr)
   return feq
```

```
###### Setup: cylindrical obstacle and velocity inlet with perturbation #######
# Creation of a mask with 1/0 values, defining the shape of the obstacle.
def obstacle_fun(x, y):
   return (x-cx) **2+(y-cy) **2<r**2
obstacle = fromfunction(obstacle fun, (nx,ny))
# Initial velocity profile: almost zero, with a slight perturbation to trigger
# the instability.
def inivel(d, x, y):
   return (1-d) * uLB * (1 + 1e-4*sin(v/lv*2*pi))
vel = fromfunction(inivel, (2,nx,ny))
# Initialization of the populations at equilibrium with the given velocity.
fin = equilibrium(1, vel)
for time in range (maxIter):
    # Right wall: outflow condition.
    fin[col3,-1,:] = fin[col3,-2,:]
    # Compute macroscopic variables, density and velocity.
    rho, u = macroscopic(fin)
    # Left wall: inflow condition.
    u[:,0,:] = vel[:,0,:]
    rho[0,:] = 1/(1-u[0,0,:]) * (sum(fin[col2,0,:], axis=0) +
                                2*sum(fin[col3.0.:], axis=0) )
    # Compute equilibrium.
    feq = equilibrium(rho, u)
    fin[[0,1,2],0,:] = feq[[0,1,2],0,:] + fin[[8,7,6],0,:] - feq[[8,7,6],0,:]
    fout = fin - omega * (fin - feg)
    # Bounce-back condition for obstacle.
    for i in range (9):
       fout[i, obstacle] = fin[8-i, obstacle]
    # Streaming step.
    for i in range (9):
       fin[i,:,:] = roll(
                          roll(fout[i,:,:], v[i,0], axis=0),
                          v[i,1], axis=1)
    # Visualization of the velocity.
    if (time%100==0):
       plt.clf()
        plt.imshow(sqrt(u[0]**2+u[1]**2).transpose(), cmap=cm.Reds)
       plt.savefig("vel.{0:03d}.png".format(time//100))
```

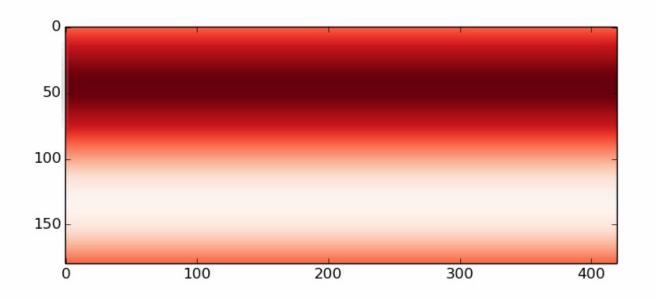
In detail: simulation parameters

```
nx, ny = 420, 180 # Number of cells r = ny//9 # Radius of obstacle uLB = 0.04 # Velocity at inlet Re = 220.0 # Reynolds number nulb = uLB*r/Re # Viscosity omega = 1 / (3*nulb+0.5) # Relax. parameter
```

Result: Re=10



Result: Re=220



End of module

Application: flow around an obstacle

End of week 5