AI Builders: 2D Fluid simulation framework via the Lattice-Boltzmann method with conditional optimizers

Puripat Thumbanthu, Kunakorn Chaiyara

Documentation written by Puripat Thumbanthu

Started: November 11, 2024; Revision: November 18, 2024

Contents

CHAPTER 1

Introduction

1.1 Backgrounds

This project, submitted to the `AI Builders X ESCK` program, originated from a series of questions.

- What's the best way to blow on a liquid filled spoon to cool it?
- Given a room, what's the best place to place an air conditioner, and what direction must it face?
- What's the best place for a cooling fan in a CPU?,

etc. These problems are a set of problems that all fall in optimization problems in fluids:

> *"Given an imposed boundary condition on a system containing fluids, a boundary condition that's free to move, and a certain function, find the boundary condition that optimizes the function."*

E.g., in the first problem, the imposed boundary condition is the shape of the room; the free boundary condition is the placement and angle of the air conditioner, and the function is the time until the room reaches thermal equilibrium.

Due to the ten weeks time limit imposed by the `AI Builders X ESCK` program. We've decided to simplify various parts of the problem to make it more fathomable.

1.2 Problem statement and overview of solution

The problem that we've selected to tackle is the second problem due to phase homogeneity: "given a room, what's the best place to place an air conditioner, and what direction must it face." Due to complexity in three-dimensions, we've decided to simplify the problem to a room with boundaries in two-dimensions, and only allow the air conditioner to exist on a line around the border of the room.

The variables that are used in this problem is as follows:

1. **The function needed for optimization**—the time until equilibrium
2. **Free boundary condition**—placement of the air conditioner, represented as a density boundary condition
3. **Imposed boundary condition**—shape of the room

It's then solved as follows:

1. Build a fluid simulator with wall and density boundary condition,
2. Input the shape of the room, and the strength of the air conditioner,
3. Find the optimal air conditioner using gradient descent.

Originally, we planned to use the `OpenFOAM` simulator, as it's commonly used by researchers in computational fluid dynamics. However, the learning curve is too steep for just ten weeks. There's no clean way to connect the data from `OpenFOAM` into `Python` for post-processing. Most importantly, there aren't many great resources out there. So, we've decided to build our own simulation and optimization algorithm from scratch using one of the most accessible methods to do fluid simulation: the Lattice-Boltzmann method.

1.3 Overview of the Lattice-Boltzmann method

The Lattice-Boltzmann method is a fluid simulation method that doesn't require discretization of the Navier-Stokes equation. Instead, it models fluids as a collection of particles in a lattice filled with cells. In each step of the simulation, the particle moves from its own cell to its adjacent cells. Then, it interacts inside the cell through self-collisions. This cell-interpretation allow the derivation of the macroscopic fluid properties, e.g., density and velocity, to be derived from the particle distributions in each lattice directly. The process includes

1. **Streaming**—particles move into adjacent cells
2. **Collisions**—the densities in each cell is adjusted towards equilibrium inside the cell.

This method is very viable for parallel computing, making it very ideal for implementation in `NumPy`. However, it is numerically unstable for high-speed fluid flows near or above the speed of sound. Since we're not dealing with particles moving that fast, we should be fine.

Even though the Lattice-Boltzmann method is stable for the most part, it still has some numerical instabilities around boundary conditions especially anything to do with circles. These will become a problem in gradient descent, in which we have to implement an algorithm to work around these instabilities.

1.3.1 Representation

Coordinate convention Since `NumPy` indexes the y-axis (vertically) before the x-axis (horizontally), all pairs of coordinates from now on is to be read as (y, x), not (x, y)

A fluid simulation with resolution $N \times M$ illustrated in fig. 1.1, is represented as a rectangular lattice with $N \times M$ cells. Each cell in the lattice contains nine cell-invariant unit vectors, $\mathbf{e}_0$ to $\mathbf{e}_8$, which represents the eight possible direction that the fluid can travel in. The value for these vectors, respective to the Cartesian representation is given in table 1.1

Unit vector	Representation
$\mathbf{e}_0$	$\mathbf{0}$
$\mathbf{e}_1$	$\hat{\mathbf{x}}$
$\mathbf{e}_2$	$\hat{\mathbf{y}}$
$\mathbf{e}_3$	$-\hat{\mathbf{x}}$
$\mathbf{e}_4$	$-\hat{\mathbf{y}}$
$\mathbf{e}_5$	$\hat{\mathbf{x}} + \hat{\mathbf{y}}$
$\mathbf{e}_6$	$-\hat{\mathbf{x}} + \hat{\mathbf{y}}$
$\mathbf{e}_7$	$-\hat{\mathbf{x}} - \hat{\mathbf{y}}$
$\mathbf{e}_8$	$\hat{\mathbf{x}} - \hat{\mathbf{y}}$

TABLE 1.1 | UNIT VECTORS USED IN A CELL OF FLUID

From the set of vectors $\mathbf{e}_0, \ldots, \mathbf{e}_8$ inside each cell, one respectively assign another set of vectors $\mathbf{f}_0, \ldots, \mathbf{f}_8$. These vectors are scaled version of

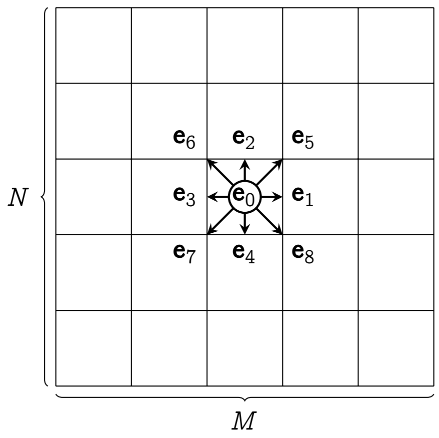


FIG. 1.1 | LATTICE OF FLUID

the unit vectors, i.e.,

$$\mathbf{f}_i = f_i \mathbf{e}_i, \tag{1.1}$$

where the scalar f_n represents the amount of fluid that's moving in the direction $\mathbf{e}_n$. From this representation alone, the density, momentum, and speed of the fluid at a certain point (n, m) can be found. The density of fluid at the cell (n, m), $\rho(n, m)$, is the sum from of all f_i's inside the cell:

$$\rho(n, m) \equiv \sum_i f_i(n, m). \tag{1.2}$$

The momentum density, $\mathbf{U}(n, m)$, traditionally given by the product between velocity and mass, can be calculated as the sum of product between f_n and their respective unit vectors:

$$\mathbf{U}(n, m) \equiv \sum_n f_n \mathbf{e}_n. \tag{1.3}$$

The velocity density at a certain cell is just the ratio between the momentum density and the fluid density:

$$\mathbf{u}(n, m) \equiv \frac{\mathbf{U}(n, m)}{\rho(n, m)} = \frac{\sum_n f_n \mathbf{e}_n}{\rho}. \tag{1.4}$$

1.3.2 Self-collision step

The self-collision step represents the relaxation of fluid that happens inside a cell. In each of the fluid vectors $\mathbf{f}_0, \dots, \mathbf{f}_8$, a corresponding equilibrium vector is assigned by

$$\mathbf{E}_i(n,m) = w_i \rho \left(1 + 3\mathbf{e}_i \cdot \mathbf{u}(n,m) + \frac{9}{2}\left(\mathbf{e}_i \cdot \mathbf{u}(n,m)\right)^2 - \frac{3}{2}|\mathbf{u}(n,m)|^2\right)\mathbf{e}_i \tag{1.5}$$

where w_i is a weighting factor that's given by the reduction of Boltzmann's distribution:

$$w_i = \begin{cases} \frac{4}{9} & \text{if } i = 0, \\ \frac{1}{9} & \text{if } i = 1,2,3,4, \\ \frac{1}{36} & \text{if } i = 5,6,7,8. \end{cases} \tag{1.6}$$

The corresponding equilibrium scalar $E_i(n,m)$, is given by the relation

$$\mathbf{E}_i(n,m) = E_i(n,m)\mathbf{e}_i. \tag{1.7}$$

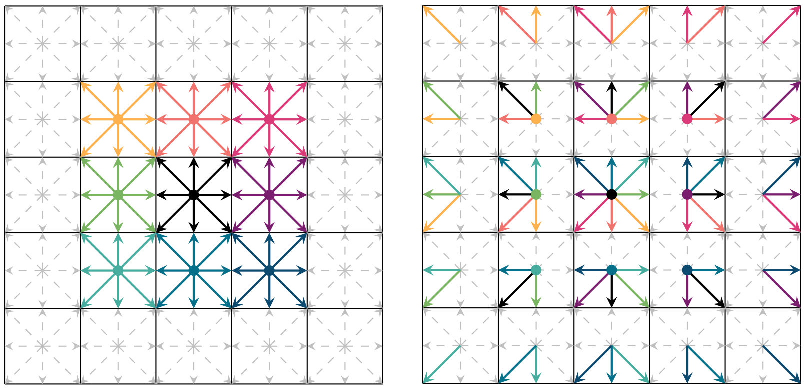
However, a fluid cannot possibly reach its own equilibrium in just one step; therefore, the Lattice-Boltzmann adjusts the fluid vector to approach the equilibrium vector. This behavior is captured by the relaxation time τ. For the set of fluid vector positioned at the cell (n,m) at time t, $f_i(n,m;t)$, the fluid vector at the next time step, $t + \Delta t$ is given by

$$f_i(n,m;t+\Delta t) = f_i(n,m;t) + \frac{1}{\tau}\left(E_i(n,m;t) - f_i(n,m;t)\right), \tag{1.8}$$

and that

$$\mathbf{f}_i(n,m;t+\Delta t) = f_i(n,m;t+\Delta t)\mathbf{e}_i. \tag{1.9}$$

The relaxation value that's used throughout this project is $\tau = 0.8070$, which is said to be the most numerically stable [8].



(A) BEFORE (B) AFTER

FIG. 1.2 | FLUID VECTORS BEFORE AND AFTER THE STREAMING STEP HIGHLIGHTED IN COLOR. GRAY VECTORS ARE NOT CONSIDERED.

1.3.3 Streaming step

Using the vector that's adjusted to the equilibrium from the self-collision step, that vector is streamed to the adjacent cells, given by

$$\mathbf{f}_i\left(n + (\hat{\mathbf{y}} \cdot \mathbf{e}_i), m + (\hat{\mathbf{x}} \cdot \mathbf{e}_i)\right) = \mathbf{f}_i(n, m; t + \Delta t). \tag{1.10}$$

Basically, this equation moves the fluid from one cell to the other as illustrated in fig. 1.2

1.3.4 Boundary conditions

There are two boundaries condition that needs to be implemented in this problem: wall and density. Since we want this to be a complete framework for two-dimensional fluid simulation, we also implemented the density boundary condition for completeness' sake.

Directional density boundary condition This boundary condition can be achieved by explicitly setting the value of f_0 to f_8 after a complete simulation step.

Wall boundary condition This boundary condition is sometimes referred off as the bounce-back boundary condition. If the fluid from an adjacent cell is streamed into a wall located at (n, m), the wall simply reflects the fluid vector back:

$$f_j\big(n - (\mathbf{e}_i \cdot \hat{\mathbf{y}}), m - (\mathbf{e}_i \cdot \hat{\mathbf{x}})\big) = f_i(n, m) \tag{1.11}$$

where

$$j = \begin{cases} i + 2 & \text{if } i = 1, 2, 5, 6, \\ i - 2 & \text{if } i = 3, 4, 7, 8. \end{cases} \tag{1.12}$$

Since the fluid cannot possibly stream into the center of the wall, j doesn't have to be defined at $i = 0$. [1]

Wall-velocity boundary condition Given a wall that's located at position (n, m), and an exposed fluid cell located at position $\big(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\big)$, the velocity boundary condition can be defined by two variables: velocity along $\mathbf{e}_a$, and along its clockwise perpendicular, $\mathbf{e}_b$ where

$$b = \begin{cases} a + 3 & \text{if } a = 1, \\ a - 1 & \text{if } a + 2, 3, 4. \end{cases} \tag{1.13}$$

Here, we define the other directions that are relative to direction a:

$$\alpha = \begin{cases} a + 2 & \text{if } a = 1, 2, \\ a - 2 & \text{if } a = 3, 4, \end{cases} \tag{1.14}$$

$$\beta = \begin{cases} a + 1 & \text{if } a = 1, 2, 3, \\ a - 3 & \text{if } a = 4, \end{cases} \tag{1.15}$$

$$A = \begin{cases} a + 7 & \text{if } a = 1, \\ a + 3 & \text{if } a = 2, 3, 4, \end{cases} \tag{1.16}$$

$$B = \begin{cases} a+6 & \text{if } a = 1,2, \\ a+2 & \text{if } a = 3,4, \end{cases} \tag{1.17}$$

$$C = \begin{cases} a+5 & \text{if } a = 1,2,3, \\ a-1 & \text{if } a = 4, \end{cases} \tag{1.18}$$

$$D = a + 4. \tag{1.19}$$

These directions live on a grid relative to direction a as illustrated in fig. 1.3.

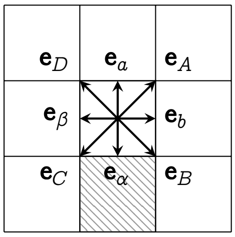


Fig. 1.3 | Directions relative to the convention given by the wall-velocity boundary condition. The shaded region is the wall, and the cell with vector arrows is the target cell in which wall-velocity boundary condition is applied.

a	b	α	β	A	B	C	D
1	4	3	2	8	7	6	5
2	1	4	3	5	8	7	6
3	2	1	4	6	5	8	7
4	3	2	1	7	6	5	8

Table 1.2 | Directions relative to the convention given by the wall-velocity boundary condition.

Given that

$$\mathbf{u}_a\left(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\right) \quad \text{and,} \quad \mathbf{u}_b\left(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\right) \tag{1.20}$$

is fixed by the boundary condition, the surrounding velocities in the cell $\big(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\big)$ can be updated as follows: [9]

$$\mathbf{f}_a = \mathbf{f}_\alpha + \frac{2}{3}\rho\big(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\big)\mathbf{f}_a, \tag{1.21}$$

$$\mathbf{f}_A = \mathbf{f}_C - \frac{1}{2}\big(\mathbf{f}_b - \mathbf{f}_\beta\big) + \rho\big(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\big)\Big(\frac{\mathbf{u}_b}{6} + \frac{\mathbf{u}_a}{6}\Big), \tag{1.22}$$

$$\mathbf{f}_D = \mathbf{f}_B - \frac{1}{2}\big(\mathbf{f}_b - \mathbf{f}_\beta\big) + \rho\big(n + (\mathbf{e}_a \cdot \hat{\mathbf{y}}), m + (\mathbf{e}_b \cdot \hat{\mathbf{x}})\big)\Big(-\frac{\mathbf{u}_b}{6} + \frac{\mathbf{u}_a}{6}\Big). \tag{1.23}$$

For the rest of the directions, use the wall boundary condition (bounce-back) to calculate the fluids vector.

CHAPTER 2

Building the simulation framework

The implementation of the model in `Python` is different from the theoretical model due to some `NumPy` functions. This chapter serves as an overview for self-implementing the model. The codes in this chapter are not the actual code used in the `GitHub` repository. It's liberated from the object-oriented paradigms for ease of understanding. All of these will be pieced together in chapter 3

This idea of implementing the simulation is actually an amalgamation of various ones. The article by Adams [1] and Schroeder [7] gave us a very comprehensive overview of the Lattice-Boltzmann method with boundaries condition, and also provided us with the intuition for creating our own ways of implementing. The inspiration for using the roll function is from Matias Ortiz's video on Lattice-Boltzmann simulator [4]. However, that video is quite old and uses a rather strange technique of implementing the boundary conditions, which leads to many numerical instabilities.

Most of the time that's spent on this project is to make the boundary condition work. At the end, it did work, with the by product of sweat and tears. We don't want anyone to suffer through them with us. So, here is how we did it.

2.1 Preliminary quantities

The packages that are used throughout the project are imported as follows:

```python
import numpy as np
import matplotlib.pyplot as plt
import itertools as itr
from scipy.ndimage import convolve
import copy
import random
import math
```

And, here are the invariant arrays that are used throughout the project:

```python
unitVect = np.array(
    [
        [0, 0], [1, 0], [0, 1],
        [-1, 0], [0, -1], [1, 1],
        [-1, 1], [-1, -1], [1, -1]
    ]
)
unitX = np.array([0, 1, 0, -1, 0, 1, -1, -1, 1])
```

```python
unitY = np.array([0, 0, 1, 0, -1, 1, 1, -1, -1])
weight = np.array([4/9, 1/9, 1/9, 1/9, 1/9, 1/36, 1/36, 1/36, 1/36])
```

The `unitVect` array represents the set of vectors $\mathbf{e}_i$ where $i = 1, 2, 3, \ldots, 8$. `unitY` and `unitX` represents $\mathbf{e}_i \cdot \hat{\mathbf{y}}$ and $\mathbf{e}_i \cdot \hat{\mathbf{x}}$ respectively. Lastly, the `weight` array represents the weight that's used to calculate the fluid equilibrium ($\mathbf{E}_i$) in eqs. (1.5), (1.6) and (1.8).

2.2 Preliminary functions

2.2.1 Representation of physical quantities

The whole lattice is represented as a `NumPy` array with dimensions $(N, M, 9)$. The first axis represents the y index, second represents the x index, and the third one with nine elements represent the fluid vectors $\mathbf{f}_0, \ldots, \mathbf{f}_8$. Since these fluid vectors actually represents the amount of fluid that's travelling inside a cell, the vectors cannot be zero. Thus, the array is set to be all ones even when the fluid at rest. One can simply initialize the array as follows:

```python
yResolution = 24 # Configurable
xResolution = 36 # Configurable
fluid = np.ones(yResolution, xResolution, 9)
# The fluid array is to be modified according to the desired initial
↪  condition
initCondition = copy.deepcopy(fluid)
```

The array `initCondition` serves as a reference for plotting in the future.

For simplicity, we also define two arrays that are used throughout: `yIndex` and `xIndex`. They are arrays that are filled with numbers from 0 to $y - 1$, and 0 to $x - 1$ respectively.

```
yIndex = np.arange(yResolution)
xIndex = np.arange(xResolution)
```

In the simulation step that is documented later in section 2.3, there must be a function that updates the density, momentum density, and velocity density of the fluid every time the simulation runs. First, we initialize the arrays that contain the density, momentum density, and the velocity density of the fluid according to eqs. (1.2) to (1.4):

```
density = np.sum(fluid, axis=2)
momentumY = np.sum(fluid * unitY, axis=2)
momentumX = np.sum(fluid * unitX, axis=2)
speedY = momentumY / density
speedX = momentumX / density
speedY = np.nan_to_num(speedY, posinf=0, neginf=0, nan=0)
speedX = np.nan_to_num(speedX, posinf=0, neginf=0, nan=0)
```

The function `np.nan_to_num` is used to deal with infinities that might occur in the velocity calculation step. At the wall boundary condition where there's no fluid there; hence, zero density. Since the velocity is the ratio between momentum and fluid density, the velocity at the wall diverges to infinity, which it really shouldn't. So, we convert those infinities to zero by using the `np.nan_to_num`.

These arrays are then updated using the following functions:

```python
def updateDensity():
    density = np.sum(fluid, axis=2)

def updateMomentum():
    momentumY = np.sum(fluid * unitY, axis=2)
    momentumX = np.sum(fluid * unitX, axis=2)

def updateSpeed():
    updateDensity()
    updateMomentum()

    speedY = momentumY / density
    speedX = momentumX / density
    speedY = np.nan_to_num(speedY, posinf=0, neginf=0, nan=0)
    speedX = np.nan_to_num(speedX, posinf=0, neginf=0, nan=0)
```

They are literally the calculation codes, but converted into a callable function. Since `updateSpeed` calls both `updateDensity` and `updateMomentum`, one doesn't have to call `updateDensity` and `updateMomentum` when the function `updateSpeed` is already called.

2.2.2 Wall boundary conditions

The wall boundaries condition is stored as another array with dimensions (N, M) filled with boolean elements. If a position (n, m) is `True`, then it is not a wall, else, it's a wall. This array can be used to easily impose the wall boundary condition on the `fluid` array. I.e., every point where there's a wall, there must be zero fluid; thus, the fluid vectors at those points shall be zero.

```python
boundary = np.full((yResolution, xResolution))
# Can be edited to be any shape desired.
fluid[boundary, :] = 0
```

There are four types of wall that's implemented in this framework: circular, border, and rectangular, and dot. Each of them can be created using their own functions.

The cylindrical wall function (`cylindricalWall`) takes in the boundary array (`boundary`), the cylinder's center (`cylinderCenter`) as a tuple in the format (y, x), and the cylinder's radius (`cylinderRadius: float`) as a floating point number, and modify the boundary array such that there's a wall with cylinder with radius `cylinderRadius` centered at the point (y, x). The implementation is as follows:

```python
def cylindricalWall(
        boundary,
        cylinderCenter: tuple, cylinderRadius: float
    ):
    for yIndex, xIndex in itr.product(
        range(yResolution), range(xResolution)
    ):
        if math.dist(cylinderCenter, [yIndex, xIndex]) ≤
        ↪  cylinderRadius:
            boundary[yIndex, xIndex] = True
```

The border wall function (`borderWall`) takes in the boundary array (`boundary`), and the thickness of the border (`thickness: int = 1`) as an integer, then modifies the boundary array such that there is a border around the simulation. This function is called to create a box surrounding the fluid.

```python
def borderWall(boundary, thickness: int = 1):
    boundary[0 : yResolution, -1 + thickness] = True
    boundary[0 : yResolution, xResolution - thickness] = True
    boundary[-1 + thickness, 0 : xResolution] = True
    boundary[yResolution - thickness, 0 : xResolution] = True
```

The rectangular wall function is used to create a rectangular wall inside the simulation. It takes in the boundary array (`boundary`) and the position of the two corner points of the rectangle (`cornerCoord1: tuple, cornerCoord2: tuple`) as a tuple in the format (y, x). It's implemented as follows:

```python
def filledStraightRectangularWall(
    boundary,
    cornerCoord1: tuple,
    cornerCoord2: tuple
):
    maxY = max(cornerCoord1[0], cornerCoord2[0])
    minY = min(cornerCoord1[0], cornerCoord2[0])
    maxX = max(cornerCoord1[1], cornerCoord2[1])
    minX = min(cornerCoord1[1], cornerCoord2[1])

    for yIndex, xIndex in itr.product(
        range(yResolution), range(yResolution)
    ):
        if (
            (xIndex ≤ maxX)
            and (xIndex ≥ minX)
            and (yIndex ≤ maxY)
            and (yIndex ≥ minY)
        ):
            boundary[yIndex, xIndex] = True
```

Lastly, the dot wall (`dotWalls`) just takes in the boundary array (`boundary`) and some coordinates, then modifies the `boundary` array so that those coordinates are walls.

```
def dotWalls(boundary, *args: tuple):
    for position in args:
        boundary[position[0], position[1]] = True
```

Since these four functions directly modifies the `boundary` array, they must be called before imposing the wall boundaries to the `fluid` array.

In some cases, it's more favorable to use the indices of the boundaries directly. The `NumPy` array can be converted to a list of indices by the function `generateIndex`. This function takes in the boundary array (`boundary`), and outputs two arrays: `boundaryIndex` and `invertedBoundaryIndex`. The `boundaryIndex` list contains the indices of walls. Invert that list, and you get the `invertedBoundaryIndex`, which contains the indices of fluids. The function is implemented as follows:

```python
def generateIndex(boundary):
    boundaryIndex = []
    invertedBoundaryIndex = []
    for i, j in itr.product(
        range(yResolution), range(xResolution)
    ):
        if boundary[i, j] != False:
            boundaryIndex.append((i, j))
        else:
            invertedBoundaryIndex.append((i, j))
    return boundaryIndex, invertedBoundaryIndex
```

Since the end goal of this project is to simulate air conditioner placements, we also have to know the possible indices that the air conditioner can end up at. Therefore, we build a function `generateACPos` that can do so:

```python
def generateACDirections(boundary):
    possibleACPos = []
    for shiftIndex, axisIndex in itr.product([-1, 1], [1, 0]):
        shiftedBoundary = np.roll(boundary, shift=shiftIndex,
         ↪  axis=axisIndex)
        possibleACPos = np.logical_or(
            possibleACPos,
            np.logical_not(boundary) & shiftedBoundary
        )
    return possibleACPos
```

This function takes in a boundary array (`boundary`) and return a list of possible air conditioner positions (`possibleACPos`). It works by shifting the `boundary` array along the four cardinal directions ($i = 1, 2, 3, 4$) by using the `np.roll` function. Then, comparing the shifted array to the original array. If a point (n, m) in the original array isn't a wall, but the point (n, m) on the shifted array along direction i isn't a wall, then an air conditioner that faces direction i can be put at point (n, m). All the possible points from all directions are combined using `np.logical_or` to obtain an array that contains all the point that can hold an air conditioner (`possibleACPos`).

Another requirement for gradient descent is that the parameters must be continuous; therefore, one must be able to stretch the two-dimensional contour of the possible air conditioner positions into a line. The function `indexPossibleACPos` will do just that. It's implemented doing breadth first search along a line until it comes back, or that the line terminates.

```
def indexPossibleACPos(possibleACPos, clear: bool = False):
    testArray = copy.deepcopy(possibleACPos)
    currentIndex = tuple()
    for yIndex, xIndex in itr.product(
        range(yResolution), range(xResolution)
    ):
        if testArray[yIndex, xIndex]:
            currentIndex = (yIndex, xIndex)
            break

    while testArray[currentIndex]:
        for latticeIndex in [1, 2, 3, 4, 5, 6, 7, 8, 0]:
            nextIndex = addTuple(
                currentIndex,
                (
                    unitX[latticeIndex],
                    unitY[latticeIndex],
                ),
            )
            if testArray[nextIndex]:
                possibleACIndex.append(nextIndex)
                testArray[currentIndex] = 0
                currentIndex = nextIndex
                break
            else:
                pass
```

2.2.3 Density boundary condition

The interpretation of this boundary condition isn't really to fix a density at a certain point. Rather, it is to make a point spew out the liquids continuously; therefore, the fluid vectors can just be set explicitly after each simulation iteration. Although I want this chapter to be liberated from object-oriented programming paradigm, this one just can't. Therefore, I shall introduce a new class: the `DensityBoundary` class, which is implemented as follows:

```
class DensityBoundary:
    def __init__(self, y: int, x: int, magnitude: float, direction:
    ↪   int):
        self.y = y
        self.x = x
        self.magnitude = magnitude
        self.direction = direction
```

This class contains the position of the density boundary condition (`y` and `x`), the magnitude of density, and the direction that the density is imposed. The density boundary condition is imposed as follows:

```
velocityBoundaries = []
def imposeDensityBoundaryCondition(boundary, velocityBoundaries):
    for velocityBoundary in velocityBoundaries:
        fluid[
            velocityBoundary.y, velocityBoundary.x,
            ↪   velocityBoundary.direction
        ] = velocityBoundary.magnitude
    updateSpeed()
```

2.2.4 Wall-velocity boundary condition

The wall-velocity boundary condition is also implemented as a class (`VelocityBoundary`) which is initialized with the (y, x) position of the boundary condition, and the velocity along direction $\mathbf{e}_a, \mathbf{e}_b$. It's implemented as follows:

```python
class VelocityBoundary:
    indices = [[1, 8, 5], [2, 5, 6], [3, 6, 7], [4, 7, 8]]

    def __init__(self, y: int, x: int, ux, uy, direction: int):
        self.y = y
        self.x = x
        self.uy = uy
        self.ux = ux
        self.direction = direction

        # For calculating the ua and ub
        reflectIndex = (direction - 2) if (direction in [3, 4]) else
        ↪  (direction + 2)

        self.mainVelocity = ux if (direction in [1, 3]) else uy
        self.minorVelocity = uy if (direction in [1, 3]) else ux
        self.setIndices = VelocityBoundary.indices[direction - 1]
        self.getIndices = VelocityBoundary.indices[reflectIndex - 1]
```

All the velocity boundaries point are then stored as an object of the class `VelocityBoundaries` in a list called `velocityBoundaries`. We then iterate over the list to update the fluid simulation grid according to eqs. (1.21) to (1.23).

```python
velocityBoundaries = [] # A list of pressure boundaries point
def imposeVelocityBoundaryCondition(fluid, velocityBoundaries):
    for velocityBoundary in velocityBoundaries:
```

```
    for latticeIndex in range(9):
        fluid[velocityBoundary.y, pressureBoundary.x, latticeIndex]
        ↪   = 0
    densityAtIndex = density[velocityBoundary.y, pressureBoundary.x]
    fluid[
        velocityBoundary.y, pressureBoundary.x,
        ↪   pressureBoundary.setIndices[0]
    ] = fluid[
        velocityBoundary.y, pressureBoundary.x,
        ↪   pressureBoundary.getIndices[0]
    ] + (
        2 / 3
    ) * (
        velocityBoundary.mainVelocity
    )
    fluid[
        velocityBoundary.y, velocityBoundary.x,
        ↪   velocityBoundary.setIndices[1]
    ] = (
        fluid[
            velocityBoundary.y,
            velocityBoundary.x,
            velocityBoundary.getIndices[1],
        ]
        - (
            0.5
            * (
                    fluid[
                        velocityBoundary.y,
                        velocityBoundary.x,
                        (
                            4
                            if velocityBoundary.direction - 1 == 0
                            else velocityBoundary.direction - 1
                        ),
                    ]
                    - fluid[
                        velocityBoundary.y,
                        velocityBoundary.x,
                        (
                            1
                            if velocityBoundary.direction + 1 == 5
                            else velocityBoundary.direction + 1
                        ),
                    ]
                )
            )
            + (0.5 * densityAtIndex * velocityBoundary.minorVelocity)
            + (1 / 6 * densityAtIndex * velocityBoundary.mainVelocity)
        )
        fluid[
            velocityBoundary.y, velocityBoundary.x, velocityBoundary.setIndices[2]
        ] = (
            fluid[
                velocityBoundary.y,
                velocityBoundary.x,
                velocityBoundary.getIndices[2],
            ]
            + (
                0.5
                * (
                    self.fluid[
                        velocityBoundary.y,
                        velocityBoundary.x,
                        (
                            4
                            if velocityBoundary.direction - 1 == 0
                            else velocityBoundary.direction - 1
                        ),
                    ]
                    - self.fluid[
                        velocityBoundary.y,
                        velocityBoundary.x,
                        (
                            1
                            if velocityBoundary.direction + 1 == 5
                            else velocityBoundary.direction + 1
                        ),
                    ]
                )
            )
            - (0.5 * densityAtIndex * velocityBoundary.minorVelocity)
            + (1 / 6 * densityAtIndex * velocityBoundary.mainVelocity)
        )
```

2.3 Simulation functions

There are three functions that are used: `streamFluid`, `bounceBackFluid`, and `collideFluid`. All of which follows the main steps of the Lattice-Boltzmann method: streaming, self-collision, and wall boundary.

Streaming step Earlier, we calculated the value of $\mathbf{e}_i \cdot \hat{\mathbf{y}}$ and $\mathbf{e}_i \cdot \hat{\mathbf{x}}$, and stored it into the array `unitX` and `unitY`. These quantities are then used to shift the array in their respective directions, representing the streaming step.

```python
def streamFluid(fluid):
    for latticeIndex, shiftY, shiftX in zip(range(9), unitY, unitX):
        fluid[:, :, latticeIndex] = np.roll(
            fluid[:, :, latticeIndex], shiftY, axis=0
        )
        fluid[:, :, latticeIndex] = np.roll(
            fluid[:, :, latticeIndex], shiftX, axis=1
        )
```

Self-collision step The code follows from eqs. (1.5) and (1.8). It iterates through every fluid vectors in a lattice and update them accordingly.

```python
def collideFluid(fluid):
    fluidEquilibrium = np.zeros(fluid.shape)
    for latticeIndex, cy, cx, w in zip(
        range(9), unitY, unitX, weight,
    ):
        fluidEquilibrium[:, :, latticeIndex] = (
            density
            * w
            * (
                1
                + 3 * (cx * speedX + cy * speedY)
                + 9 * (cx * speedX + cy * speedY) ** 2 / 2
                - 3 * (speedX**2 + speedY**2) / 2
            )
        )
    fluid += (fluidEquilibrium - fluid) / relaxationTime
```

Imposing wall boundary condition We define a dictionary `reflectIndices` to convert from the index that's pointing into the wall to the index that points opposing the wall. The elements of the dictionary directly reflect the relation given by eq. (1.12). The part that updates the fluid directly reflects eq. (1.11).

```python
boundaryIndex, invertedBoundaryIndex = generateIndex(boundary)
reflectIndices = {0: 0, 1: 3, 2: 4, 3: 1, 4: 2, 5: 7, 6: 8, 7: 5, 8: 6}
def bounceBackFluid(fluid):
    for y, x in boundaryIndex:
        for latticeIndex in range(9):
            if fluid[y, x, latticeIndex] != 0:
                bounceIndexY = y - unitY[latticeIndex]
                bounceIndexX = x - unitX[latticeIndex]
                if (bounceIndexY ≥ 0 and bounceIndexY < yResolution) and (
                    bounceIndexX ≥ 0 and bounceIndexX < xResolution
                ):
                    fluid[
                        bounceIndexY,
                        bounceIndexX,
                        reflectIndices[latticeIndex],
                    ] = fluid[y, x, latticeIndex]
                    fluid[y, x, latticeIndex] = 0
    updateSpeed()
```

2.4 Simulation loop

We first define a counter that counts the amount of times that we ran the simulation: `step`. For further comparison, we deep-copy the state of the fluid before updating to the variable `lastStepFluid`. Then, the fluid vector is updated in order: stream, bounce back, self-collide, impose velocity, and impose density.

```python
step = 1
def stepSimulation(fluid):
    lastStepFluid = copy.deepcopy(fluid)
    streamFluid()
    bounceBackFluid()
    collideFluid()
    imposeVelocityBoundaryCondition()
    imposePressureBoundaryCondition()
    step += 1
```

Then, another function is implemented as a way to loop over the step function:

```python
def simulate(fluid, step: int = 1):
    [stepSimulation(fluid) for i in range(step)]
```

2.5 Metrics and baseline function

A more explicit form of the problem is

Find the air conditioner position that makes the system reaches the equilibrium the fastest.

So, it's necessary to have a function that will simulate the fluid until equilibrium. Here, the word *equilibrium* is defined as the point in which the difference in the sum of fluid vector between the last simulation step (`lastStepFluid`), and the current step (`fluid`), is smaller than a set threshold (`equilibriumThreshold`), which is normally set to be 0.5. The function that determines whether the system has reached equilibrium or not is called `isEquilibrium`. This function takes in a fluid state and its past state, then outputs a boolean. If it's true, then the system has reached equilibrium, otherwise, it hasn't.

```python
def isAtDensityEquilibirum(
    fluid, lastStepFluid, threshold: float = 0.5
):
    error = np.sum(np.abs(self.lastStepFluid - self.fluid))
    return not (error ≥ threshold)
```

The function to simulate until equilibrium also needs some care. Firstly, some initial condition where the simulation is numerically unstable, so the simulation has to be terminated before it uses up all the memory. This can be done by terminating the simulation when the sum of the fluid vectors reaches a certain threshold: the `explodeThreshold`. Secondly, some initial condition isn't numerically unstable, but doesn't reach an equilibrium either, so the amount of simulation passes limit (`limit`) must be set to control how many steps the simulation can take before forcing it to terminate. Altogether, the `simulateUntilEquilibrium` function is implemented as follows:

```python
def simulateUntilEquilibrium(
    fluid,
    limit: int = 5000,
    equilibriumThreshold: float = 0.5,
    explodeThreshold: float = 11 * xResolution * yResolution,
):
    step = 0
    isStable = True
    for _ in range(limit):
        stepSimulation()
        step += 1
        if np.sum(self.fluid) > explodeThreshold:
            isStable = False
            break
        if isAtDensityEquilibirum(equilibriumThreshold):
            break

    return step, isStable
```

2.6 Plotting the results

Plotting various aspects of the fluid simulation is quite straightforward with the framework that we've built. The density plot can be achieved directly by using the `imshow` function. [5]

```
plt.imshow(density, cmap="hot", interpolation="hermite")
```

where `cmap` is the color map, and `interpolation` is the color map smoothing algorithm. The full list of options for both of these can be found in Matplotlib's documentation: [2] (`cmap`), and [3] (`interpolation`).

The momentum density and the velocity density can be directly plotted along with the **quiver** function from Matplotlib. [6]

```python
fig, ax = plt.subplots()
heatmap = ax.imshow(
    densityPlot, cmap = "hot", interpolation = "hermite"
)
quivermap = ax.quiver(xIndex, yIndex, momentumX, -momentumY)
# Change momentumX, -momentumY to speedX, and speedY to plot the
↪  velocity instead of momentum.
fig.colorbar(heatmap)
plt.show()
```

The `momentumY` has to have a negative sign upfront because `matplotlib` libraries doesn't invert the y and x axes like the `NumPy` convention. Further modifications of the plot can be found in Matplotlib's quiver documentation: [6].

CHAPTER 3

Framework structure

As said, we shall enforce the object-oriented paradigm of `Python` by turning everything into an object one by one

3.1 Class `WallBoundary`

The `WallBoundary` class is used to store the position of walls, and is initialized with the following variables

- `yResolution: int`
- `xResolution: int`
- `invert: bool = False`

Along with these constants that are baked into the class

```python
class WallBoundary:
    unitVect = np.array(
        [
            [0, 0], [1, 0], [0, 1],
            [-1, 0], [0, -1], [1, 1],
            [-1, 1], [-1, -1], [1, -1]
        ]
    )
    unitX = np.array([0, 1, 0, -1, 0, 1, -1, -1, 1])
    unitY = np.array([0, 0, 1, 0, -1, 1, 1, -1, -1])
    directions = [
        (1, -1), (1, 1), (1, 1), (-1, 1),
        (1, -1), (1, 1), (-1, 1), (-1, -1)
    ]
```

The `invert` variable is used in case the walls needed to be inverted. E.g., instead of generating a cylinder in the middle, we want the cylinder to enclose the fluid instead. If `invert` is true, then the wall boundaries is inverted.

The object variables are then evaluated as follows:

```
self.yResolution = yResolution
self.xResolution = xResolution
self.invert = invert
self.boundary = np.full((yResolution, xResolution), invert)
self.invertedBoundary = np.invert(self.boundary)
self.boundaryIndex = []
self.invertedBoundaryIndex = []

self.possibleACPos = np.full((yResolution, xResolution), False)
```

```
        self.possibleACIndex = []
        self.possibleACDirections = None
```

The class contains the following function.

- `generateIndex(self)`
- `generateACPos(self)`
- `indexPossibleACPos(self)`
- `cylindricalWall(self, cylinderCenter: tuple, cylinderRadius: float)`
- `filledStraightRectangularWall(self, cornerCoord1: tuple, cornerCorod2: tuple)`
- `borderWall(self, thickness: int = 1)`
- `dotWalls(self, *args: tuple)`

The top three functions are used by the simulation to generate various indices for placing the air conditioner. The lower five are used to modify the boundaries directly. All the coordinates that are used in these class functions are tuples in the form (y, x). These functions must be called before initializing the simulation using the `Simulation` class, documented in section 3.4.

3.2 Class `DensityBoundary`

This class is used to model density boundary condition and is implemented as follows:

```
class VelocityBoundary:
    def __init__(
```

```python
        self, y: int, x: int, magnitude: float, direction: int
    ):
        self.y = y
        self.x = x
        self.magnitude = magnitude
        self.direction = np.array(direction)
```

This class does not have any methods or functions.

If a simulation has multiple density boundary condition, they must be stored in a list and passed to the variable `densityBoundaries` of the `Simulation` class, documented in section 3.4.

3.3 Class `VelocityBoundary`

This class is used to model velocity boundary condition and is implemented as follows:

```python
class VelocityBoundary:
    indices = [[1, 8, 5], [2, 5, 6], [3, 6, 7], [4, 7, 8]]

    def __init__(self, y: int, x: int, ux, uy, direction: int):
        self.y = y
        self.x = x
        self.uy = uy
        self.ux = ux
        self.direction = direction
        if direction in [3, 4]:
            reflectIndex = direction - 2
        else:
            reflectIndex = direction + 2

        self.mainVelocity = ux if direction in [1, 3] else uy
        self.minorVelocity = uy if direction in [1, 3] else ux
        self.setIndices = PressureBoundary.indices[direction - 1]
        self.getIndices = PressureBoundary.indices[reflectIndex - 1]
```

If a simulation has multiple velocity boundary condition, they must be stored in a list and passed to the variable `velocityBoundaries` of the `Simulation` class, documented in section 3.4.

3.4 Class `Simulation`

The class `Simulation` is used to initialize a simulation and store all the physical variables and boundaries condition of a simulation. It's initialized with the following variables:

- `yResolution: int`
- `xResolution: int`
- `initCondition: np.array`
- `wallBoundary: WallBoundary`
- `densityBoundaries: list = []`
- `velocityBoundaries: list = []`
- `relaxationTime: float = 0.8090`
- `initialStep: int = 0`

The following constants are baked into the class:

```python
class Simulation:
    unitVect = np.array(
        [
            [0, 0], [1, 0], [0, 1],
            [-1, 0], [0, -1], [1, 1],
            [-1, 1], [-1, -1], [1, -1]
        ]
    )
    unitX = np.array([0, 1, 0, -1, 0, 1, -1, -1, 1])
    unitY = np.array([0, 0, 1, 0, -1, 1, 1, -1, -1])
    weight = np.array(
        [
            4 / 9, 1 / 9, 1 / 9, 1 / 9, 1 / 9,
            1 / 36, 1 / 36, 1 / 36, 1 / 36
        ]
    )
    latticeSize = 9
    reflectIndices = {
        0: 0, 1: 3, 2: 4, 3: 1, 4: 2, 5: 7, 6: 8, 7: 5, 8: 6
    }
```

Then, the following class variables are calculated:

```python
self.yResolution = yResolution
self.xResolution = xResolution
self.yIndex = np.arange(yResolution)
self.xIndex = np.arange(xResolution)
self.initCondition = copy.deepcopy(initCondition)
self.fluid = copy.deepcopy(initCondition)
self.lastStepFluid = initCondition
self.relaxationTime = relaxationTime
self.wallBoundary = wallBoundary
self.wallBoundary.generateIndex()
self.fluid[self.wallBoundary.boundary, :] = 0
self.pressureBoundaries = pressureBoundaries
self.velocityBoundaries = velocityBoundaries
self.step = initialStep

self.density = np.sum(self.fluid, axis=2)
self.momentumY = np.sum(self.fluid * Simulation.unitY, axis=2)
self.momentumX = np.sum(self.fluid * Simulation.unitX, axis=2)
self.speedY = self.momentumY / self.density
self.speedX = self.momentumX / self.density
self.speedY = np.nan_to_num(self.speedY, posinf=0, neginf=0, nan=0)
self.speedX = np.nan_to_num(self.speedX, posinf=0, neginf=0, nan=0)
```

The variable `initCondition` must be a `NumPy` array shaped `(yResolution, xResolution, 9)`. A wall boundary is required to initialize this class. If the simulation contains no walls, pass in an object of class `WallBoundary` (section 3.1) without calling any functions on it. Optionally, one might pass in a list of velocity boundary conditions and pressure boundary condition. A common way to initialize this class is.

```python
yResolution = 24  # Can be modified
xResolution = 36  # Can be modified
initCondition = np.ones((yResolution, xResolution,
↪  Simulation.latticeSize)) / 9
walls = WallBoundary(yResolution, xResolution)
# Call the WallBoundary class methods here to generate the desired
↪  walls.
walls.cylindricalWall((12, 10), 5) # Ex: Generate a cylinder at (12, 10)
↪  with radius 5
walls.borderWall() # Ex: Generate a border for the simulation

# Examples of density and velocity boundary conditions.
densityInlet = [DensityBoundary(12, 2, 1, 1)]
velocityInlet = [VelocityBoundary(12, 2, 1, 0, 1)]

# Initializing the simulation
simulation = Simulation(
    yResolution,
    xResolution,
    initCondition,
    walls,
    densityBoundaries = densityInlet,
    velocityBoundaries = velocityInlet
)
```

This class contains the following functions:

- `updateDensity(self)`
- `updateMomentum(self)`
- `updateSpeed(self)`
- `streamFluid(self)`
- `bounceBackFluid(self)`
- `collideFluid(self)`
- `imposeVelocityBoundaryCondition(self)`
- `imposePressureBoundaryCondition(self)`
- `stepSimulation(self)`
- `simulate(self, step: int = 1)`
- `isAtDensityEquilibrium(self, threshold: float = 0.5)`
- `simulateUntilEquilibrium(self, limit: int = 5000, equilibriumThreshold: float = 0.5, explodeThreshold: float = 400)`

CHAPTER 4

Optimization algorithm

4.1 Overview

Originally, we planned to use the stochastic gradient descent algorithm straight on the possible air conditioner position. However, it falls short because most of the best points are all scattered throughout the rooms. The time until equilibrium of most half-way point of a straight wall is mostly similar, and is the optimal position. Meaning that there are many hills and valleys in our loss function; thus, gradient descent is basically out of the window.[1]

Recognizing that the visual geometry of the room is significant to optimizing the air conditioner placement, we settled for a convolutional neural network: a machine-learning method which can easily recognize the shape of a room. The overview of the plan is as follows:

[1]It took us about four weeks before realizing that both the original gradient descent and its best cousin, `AdamW` literally doesn't work because of the room's geometry with many sharp corners. They are all smooth in its own sense, but it changes rapidly when a corner is hit.

1. Generate a data set that captures
   a) **Data**—The shape of the room in as `.png` files
   b) **Labels**—The best air conditioner position as a tuple (Y, X)
2. Import the data into a `tensorflow` compatible format, then do train-test split
3. Design the convolutional neural networks layer
4. Train the model using a Pythagorean distance loss function

4.2 Data generation algorithm

4.3 Convolutional neural networks

4.4 Discussion on the pitfalls of pure gradient descent

Bibliography

[1]V. Adams, *Lattice-boltzmann in python, c, and verilog*, https://vanhunteradams.com/DE1/Lattice_Boltzmann/Lattice_Boltzmann.html (visited on 11/15/2024).

[2]*Choosing colormaps in matplotlib — matplotlib 3.9.2 documentation*, https://matplotlib.org/stable/users/explain/colors/colormaps.html (visited on 11/17/2024).

[3]*Interpolations for imshow — matplotlib 3.9.2 documentation*, https://matplotlib.org/stable/gallery/images_contours_and_fields/interpolation_methods.html (visited on 11/17/2024).

[4]Matias Ortiz, *Simple lattice-boltzmann simulator in python | computational fluid dynamics for beginners*, Apr. 15, 2022.

[5]*Matplotlib.pyplot.imshow — matplotlib 3.9.2 documentation*, https://matplotlib.org/stable/api/_as_gen/matplotlib.pyplot.imshow.html (visited on 11/17/2024).

[6]*Matplotlib.pyplot.quiver — matplotlib 3.9.2 documentation*, https://matplotlib.org/stable/api/_as_gen/matplotlib.pyplot.quiver.html.

[7]V. Schroeder, *Lattice-boltzmann fluid dynamics, Physics 3300, weber state university, spring semester, 2012*, (2012) https://physics.weber.edu/schroeder/javacourse/LatticeBoltzmann.pdf (visited on 11/17/2024).

[8]Zhao, "Optimal relaxation collisions for lattice boltzmann methods", Computers & Mathematics with Applications **65**, 172–185 (2013).

[9]Q. Zou and X. He, "On pressure and velocity boundary conditions for the lattice boltzmann bgk model", Physics of Fluids **9**, 1591–1598 (1997).