Mushroom Cloud Simulation

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Implementation

Lattice Boltzmann modeling

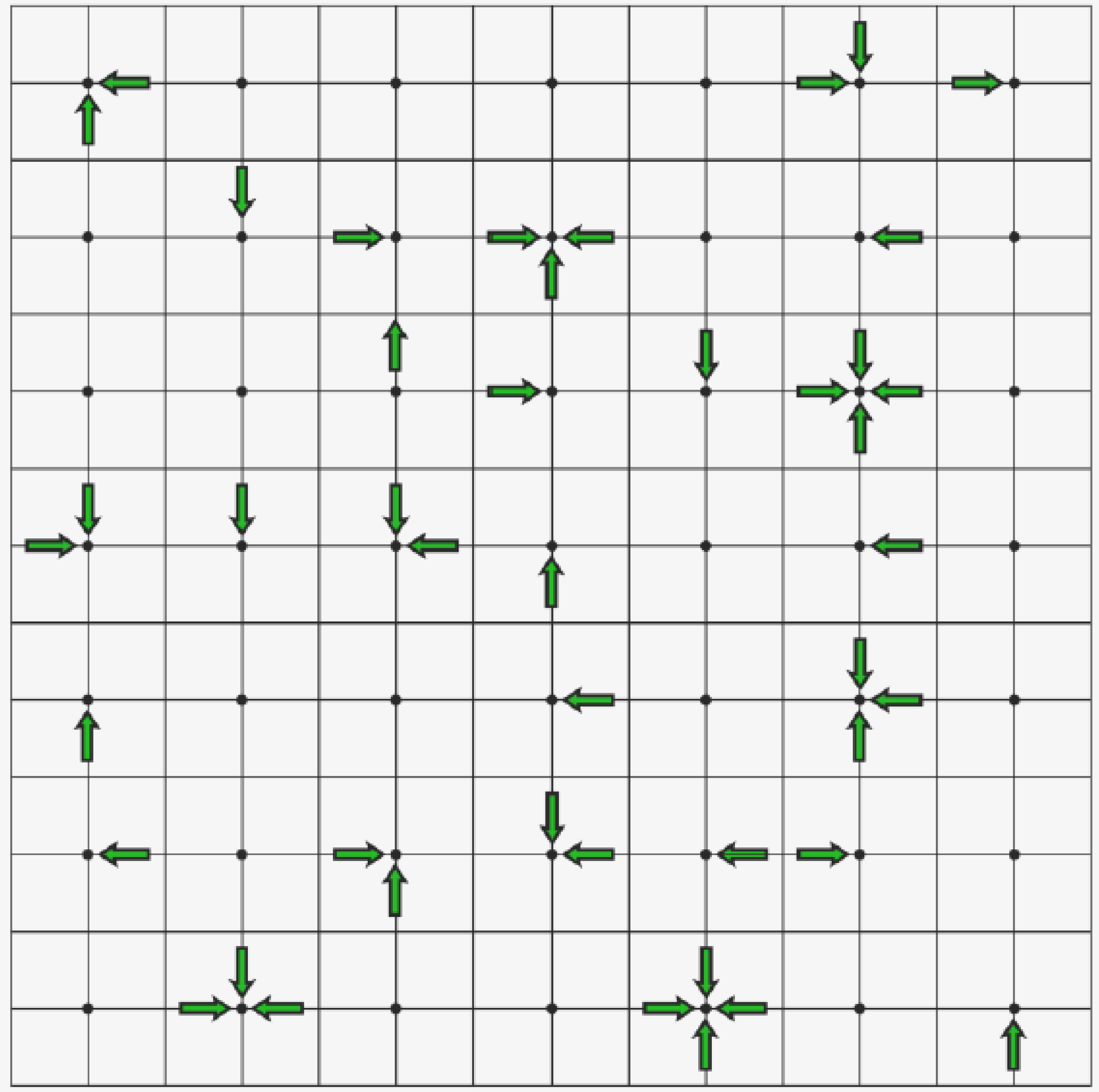
A class of computational fluid dynamics methods for fluid simulation. By simulating streaming and collision processes across a limited number of particles, the intrinsic particle interactions evince a microcosm of viscous flow behavior applicable across the greater mass.

Python/math, numpy, matplotlib

Math packages for matrices manipulation and graph plotting.

Python/vPython

VPython makes it unusually easy to write programs that generate navigable real-time 3D animations. It is based on the Python programming language.



Our Process

Incompressible Fluid
Isothermal Process
Kármán vortex street

Conduction Only

Convection only
Rayleigh–Bénard convection
(Boussinesq approximation)

2D Atomic Bombing

All about Physics

What and How - Boltzmann Equation

This equation describes the statistical behavior of a thermodynamic system not in a state of equilibrium, which arisen by considering a probability distribution for the position and momentum of a typical particle.

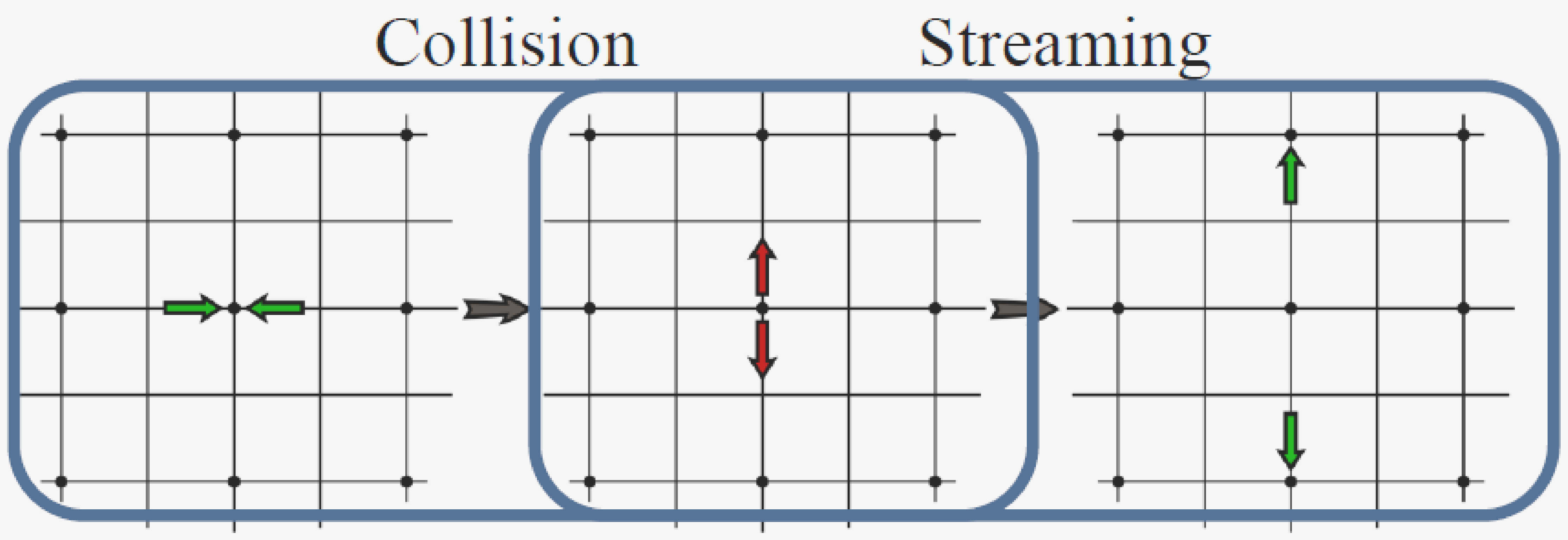
$$dN = f(\mathbf{r}, \mathbf{p}, t) d^3\mathbf{r} d^3\mathbf{p}$$

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

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

What and How - BGK Model

Since much of the challenge in solving the Boltzmann equation with the complex collision term, attempts have been made to "model" and simplify the collision term. The best known model equation is the BGK approximation.



$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \nu(f_0 - f)$$

$$\Omega_i = -\tau^{-1}(n_i - n_i^{EQ})$$

In BGK Model...

Particle/Mass Collision Term

Inspired by kinetic theory, we formulate the collision term in lattice Boltzmann as a relaxation to local equilibrium, where omega is the frequency of relaxation.

Equilibrium

The equilibrium is obtained as a truncated series of the Maxwell-Boltzmann distribution. The constants t compensate for the different lengths of velocities v.

Frequency and Viscosity

If omega is small, the fluid converges only slowly to its equilibrium: it is highly viscous. The fluid viscosity depends inversely on the relaxation parameter omega.

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

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

$$t_i = \begin{bmatrix} 1/36 & 1/9 & 1/36 \\ 1/9 & 4/9 & 1/9 \\ 1/36 & 1/9 & 1/36 \end{bmatrix}$$

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

In BGK Model (with Boussinesq approx.)/Convection

Particle/Mass Collision Term

Rayleigh-Benard convection is a type of natural convection, in which the fluid motion is not purely driven by an external force, but also by density differences in the fluid due to temperature gradients. By combining the new evolution equation and the buoyancy term, we have BGK model with temperature term.

Buoyancy Term

The coupling of the two models is established by recognizing that temperature is incorporated into as a buoyancy forcing term.

$$f_i^{out} - f_i^{in} = -\omega(f_i^{in} - E(i, \rho, \vec{u})) + b_i$$

$$b_i = -\frac{1}{2c}\triangle t \alpha_i \vec{e_i} \cdot \vec{g}\beta(T - T_0)$$

In BGK Model (with Boussinesq approx.)/Conduction

Temperature/Energy Collision Term

Rayleigh-Benard convection is a type of natural convection, in which the fluid motion is not purely driven by an external force, but also by density differences in the fluid due to temperature gradients. By combining the new evolution equation and the buoyancy term, we have BGK model with temperature term.

$$T_i(\vec{x} + c\vec{e_i}\Delta t, t + \Delta t) = T_i(\vec{x}, t) - \frac{1}{\tau'}(T_i - T_i^{eq})$$

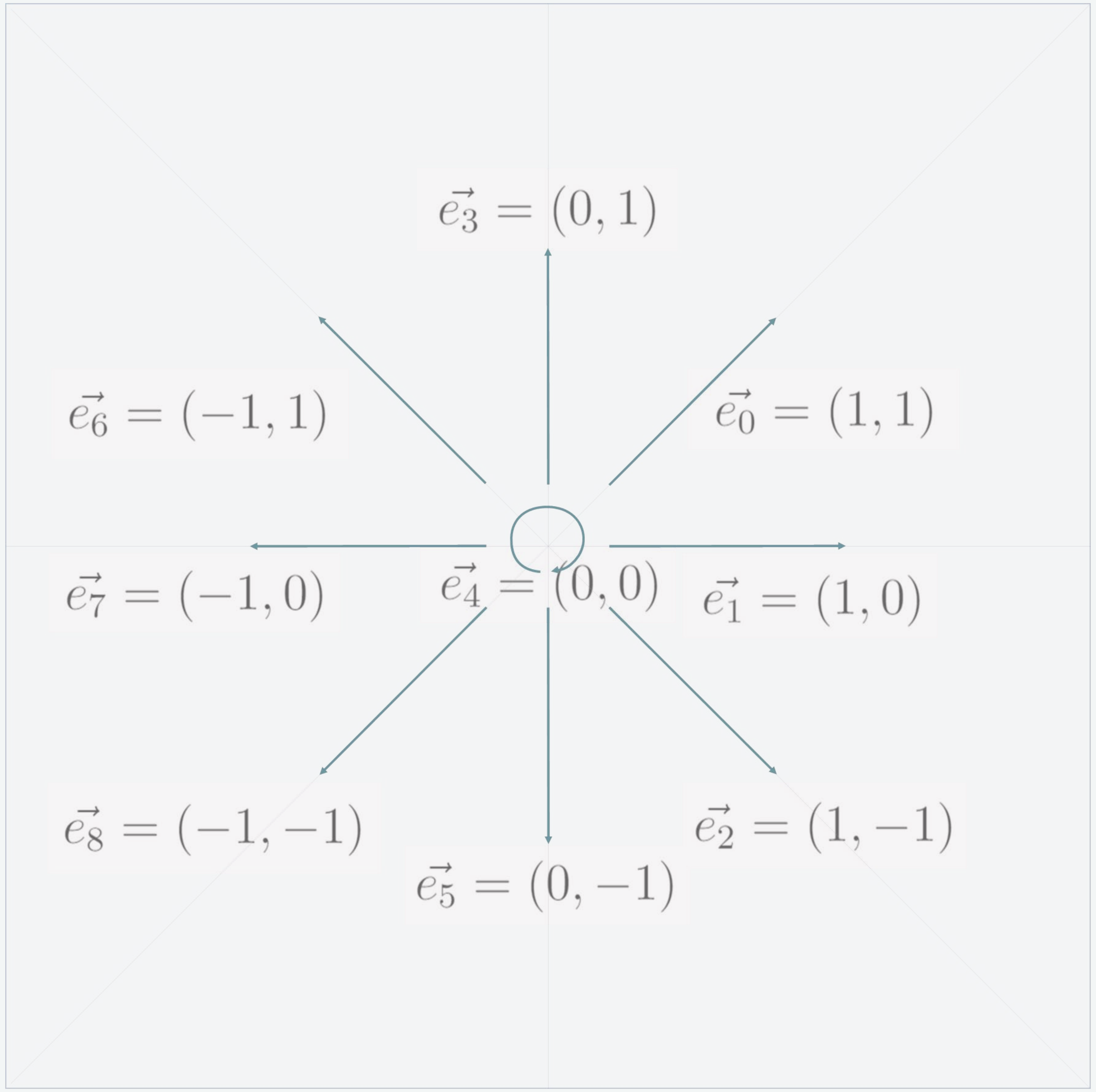
$$T_i^{eq} = \frac{T}{4}\left[1 + 2\frac{\vec{e_i} \cdot \vec{u}}{c}\right]$$

$$\kappa = \frac{2\tau' - 1}{4}\frac{(\Delta x)^2}{\Delta t}$$

while BGK in Python:

D2Q9

For a two dimensional model, a particle is restricted to stream in a possible of 9 directions, including the one staying at rest. These velocities are referred to as the microscopic velocities and denoted by $\vec{e_i}$ where i = 0..8. This model is commonly known as the D2Q9 model as it is two dimensional and involves 9 velocity vectors.



BGK/Macroscopic

Density Term

The macroscopic fluid density can be defined as a summation of microscopic particle distribution Function.

Velocity Term

Accordingly, the macroscopic velocity $\vec{u}(\vec{x},t)$is an average of microscopic velocities $\vec{e_i}$ weighted by the distribution functions f_i

Equilibrium

If omega is small, the fluid converges only slowly to its equilibrium: it is highly viscous. The fluid viscosity depends inversely on the relaxation parameter omega.

```
rho = sum(fin,axis=0)
```

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

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

$$\vec{u} = \frac{1}{\rho}\sum_{i=0}^{8} c f_i \vec{e_i}$$

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

```
def equilibrium():
    usqr = 3/2 * (u[0]**2+u[1]**2)
    feq = zeros((9,nx,ny))
    for i in range(9):
        vu = 3 * (v[i,0]*u[0,:,:]+v[i,1]*u[1,:,:])
        feq[i,:,:] = rho*weightN[i] * (1+vu+0.5*vu**2-usqr)
    return feq
```

BGK

Collision – Mass/Q9 & Temperature/Q5

Rayleigh-Benard convection is a type of natural convection, in which the fluid motion is not purely driven by an external force, but also by density differences in the fluid due to temperature gradients. By combining the new evolution equation and the buoyancy term, we have BGK model with temperature term.

$$T_i(\vec{x} + c\vec{e}_i\Delta t, t + \Delta t) = T_i(\vec{x}, t) - \frac{1}{\tau'}(T_i - T_i^{EQ})$$

$$f_i^{out} - f_i^{in} = -\omega(f_i^{in} - E(i, \rho, \vec{u})) + b_i$$

```
force = zeros((9,nx,ny))
avgT = average(T)
for i in range(9):
    force[i] = 3*weightN[i]*rho*(T-avgT)*(v[i,0]*0+v[i,1]*gr)/(Thot-Tcold)
    force[i,obstacle] = 0.0
fout = fin - omegaN * (fin - feq) + force

Tout = Tin-omegaT*(Tin-Teq)
```

Streaming

Since overwriting risks, we make stream to the neighbor and from the neighbor at the same time, exchanging populations instead of overwriting them.

$$f_i^{in}(\vec{x} + c\vec{e}_i\delta t, t + \delta t) = f_i^{out}(\vec{x}, t)$$

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

Boundary condition

Inflow/Zou-He BC

Inspired by kinetic theory, we formulate the collision term in lattice Boltzmann as a relaxation to local equilibrium, where omega is the frequency of relaxation.

Outflow

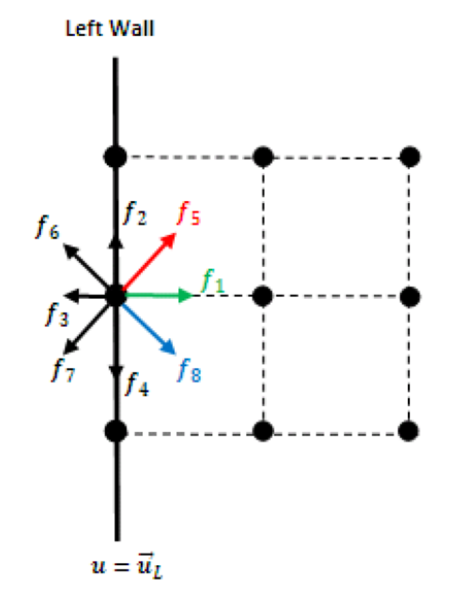
The equilibrium is obtained as a truncated series of the Maxwell-Boltzmann distribution. The constants t compensate for the different lengths of velocities v.

Obstacle/No-Slip Wall

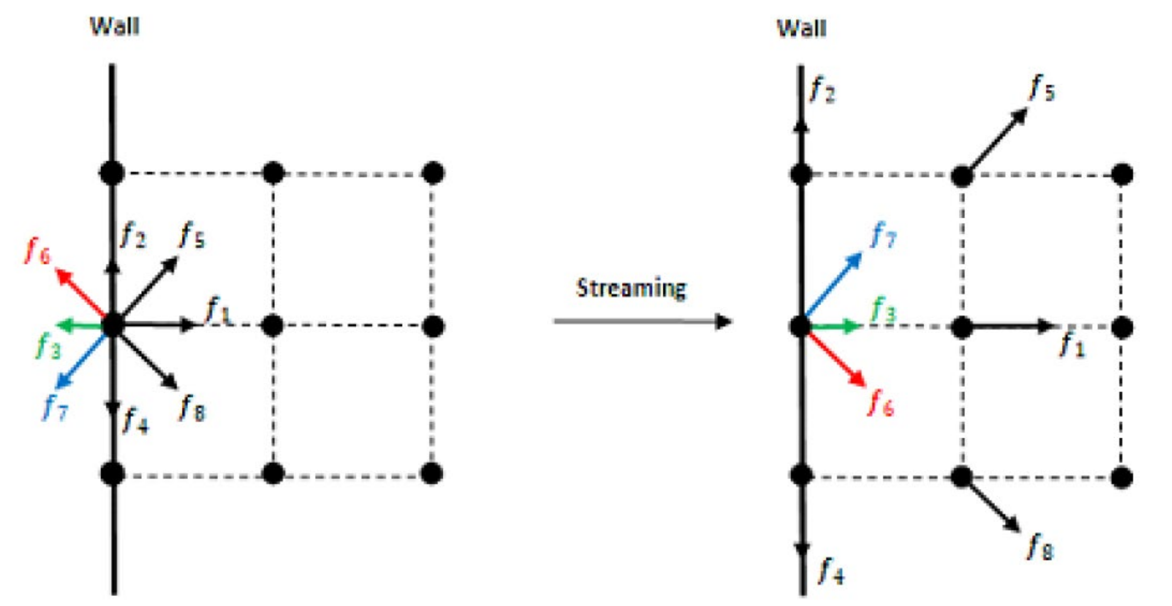
If omega is small, the fluid converges only slowly to its equilibrium: it is highly viscous. The fluid viscosity depends inversely on the relaxation parameter omega.

```
Tin[5,:,-1] = Tcold - Tin[3,:,-1] - Tin[7,:,-1] - Tin[1,:,-1] - Tin[4,:,-1]
Tin[3,:,0] = Tcold - Tin[7,:,0] - Tin[1,:,0] - Tin[5,:,0] - Tin[4,:,0]
Tin[1,0,:] = Tcold - Tin[5,0,:] - Tin[7,0,:] - Tin[3,0,:] - Tin[4,0,:]
Tin[7,-1,:] = Tcold - Tin[1,-1,:] - Tin[5,-1,:] - Tin[3,-1,:] - Tin[4,-1,:]
```

```
fin[col3,-1,:] = fin[col3,-2,:]
fin[colup,:,-1] = fin[colup,:,-2]
fin[col1,0,:] = fin[col1,1,:]
```



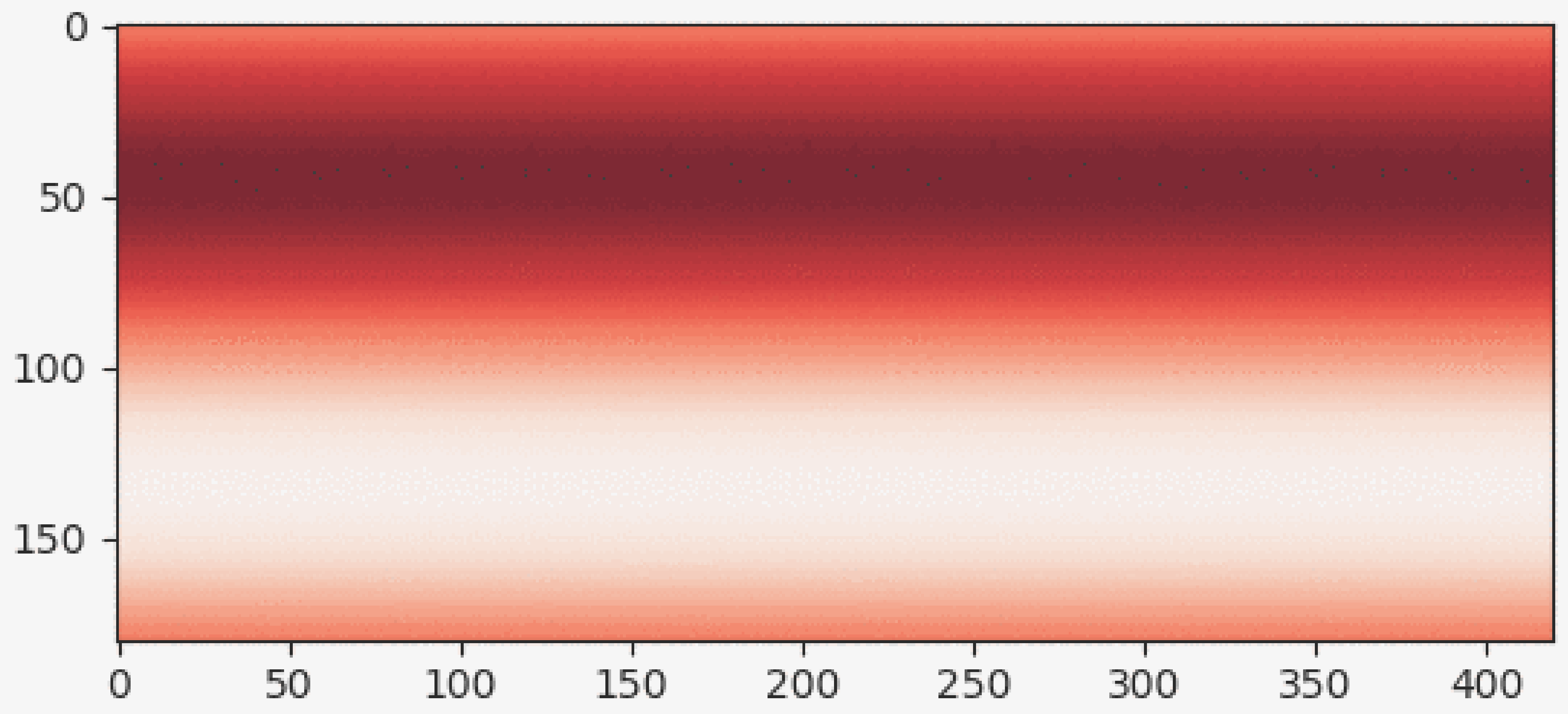

```
for i in range(9):
    fout[i,obstacle] = fin[8-i,obstacle]
```



GIFs

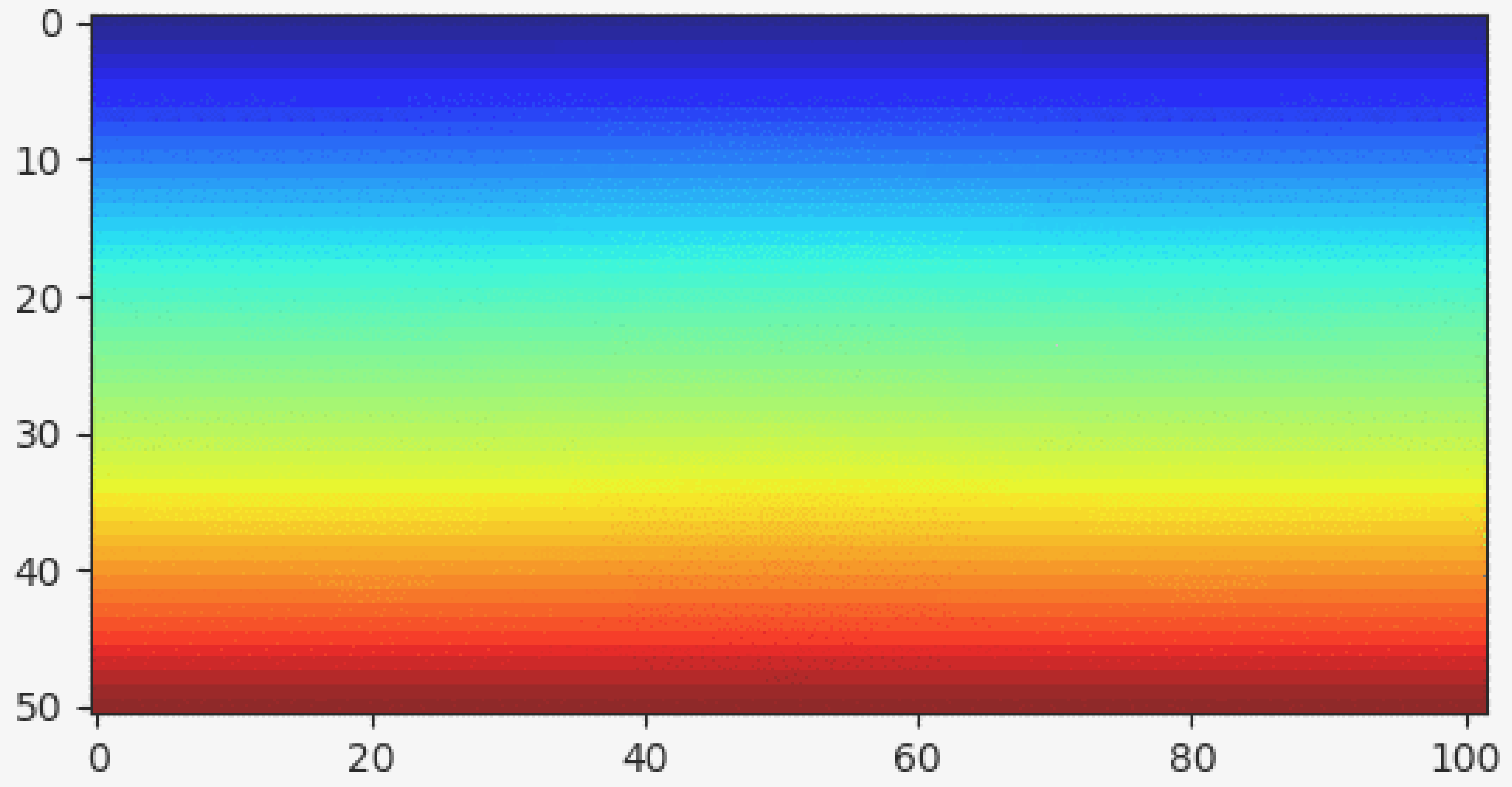
Results - Kármán vortex

The collection of screenshots that consists of the gif. Sit back and enjoy it!



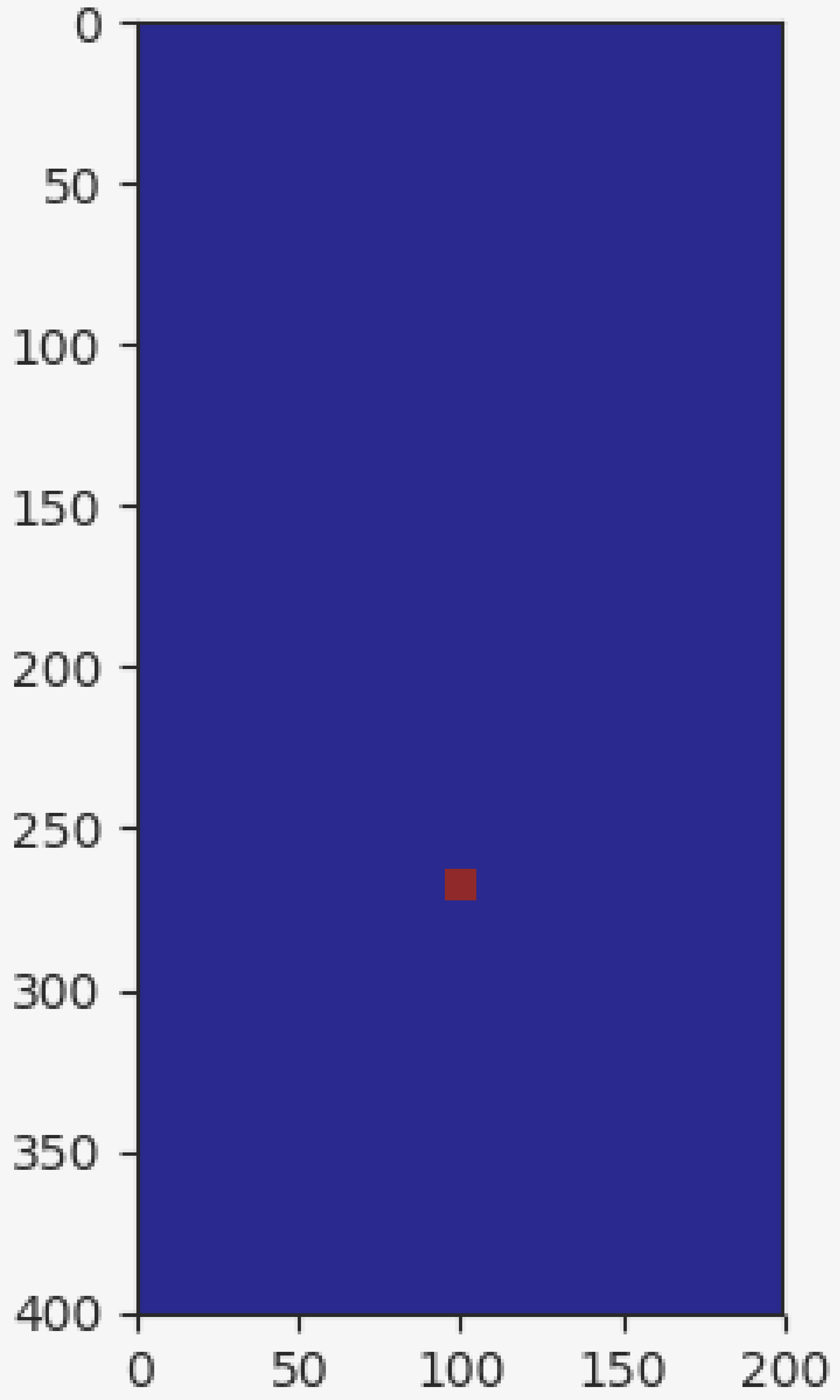
Results - Rayleigh–Bénard convection

The collection of screenshots that consists of the gif. Sit back and enjoy it!



Results - Atomic Bomb

The collection of screenshots that consists of the gif. Sit back and enjoy it!



Thanks!

Want to dig more?

See ref and visit the project at

https://github.com/ChexterWang/Mushroom

Reference

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- https://en.wikipedia.org/wiki/Lattice_Boltzmann_methods
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- https://www.coursera.org/learn/modeling-simulation-natural-processes
- https://github.com/wme7/Aero-matlab/blob/master/LBM/rayleighbenard.m