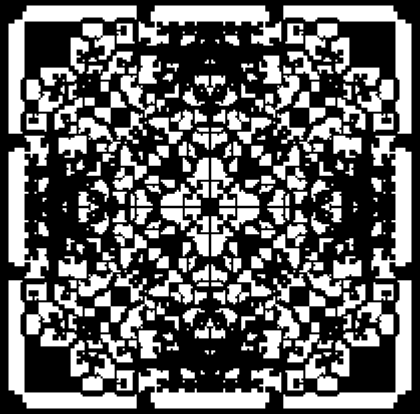
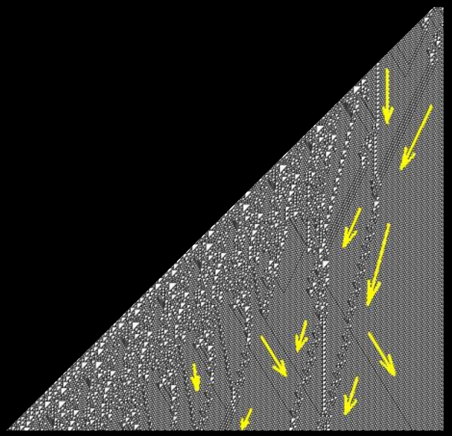
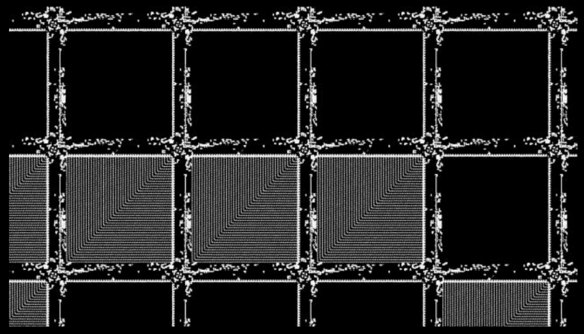
Computer modeling of physical phenomena

19-20.03.2024

Lecture IV: LBM

Cellular automata

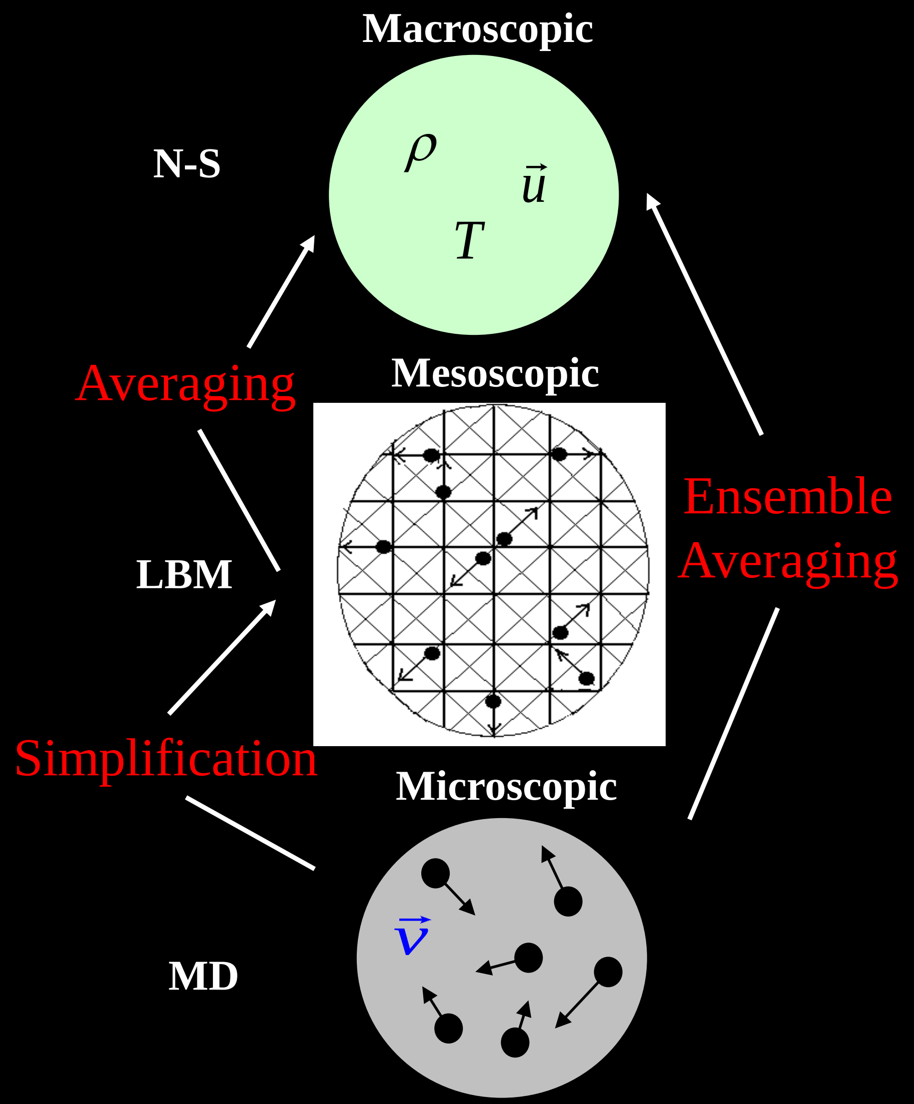
  

It’s all very nice but....

What it has to do with physics?

Lattice Gases and Lattice Boltzmann Method

Mesoscopic approach



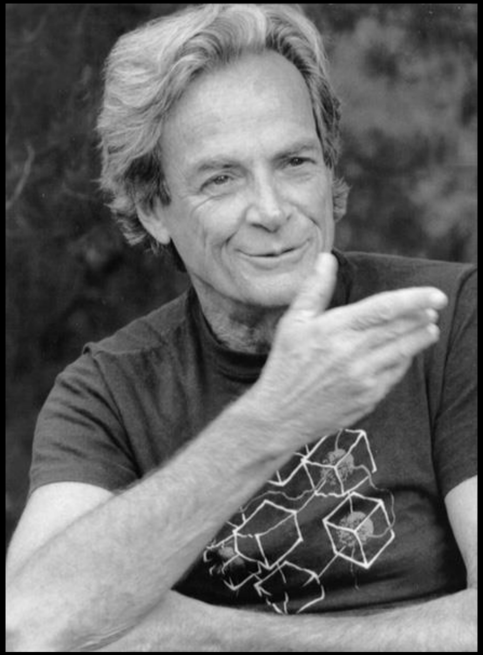
Lattice-particle methods

Idea: Solve fluid equations using fictitious particle dynamics.

Universality: Molecular details do not count as long as correct dynamics is recovered in the macroscopic limit.

Feynman on lattice automata

„We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, that flow of sand is very similar to the flow of water…"

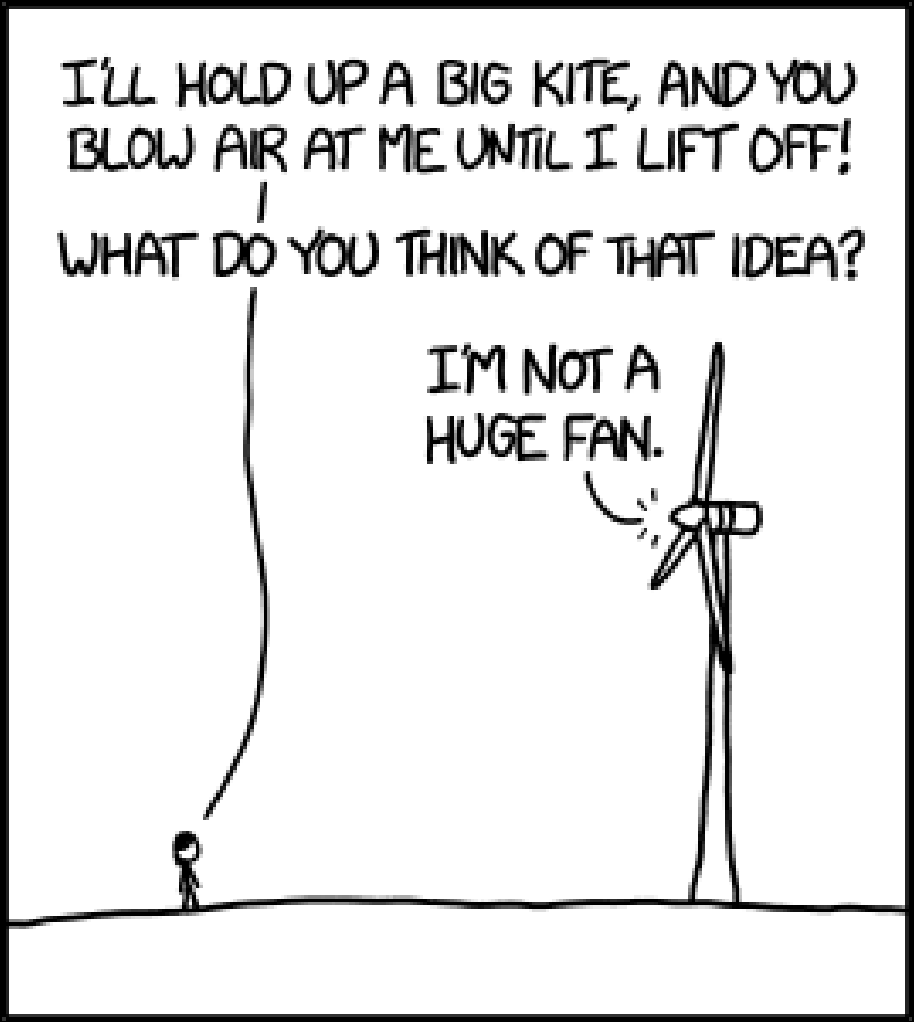


https://longnow.org/essays/richard-feynman-connection-machine/

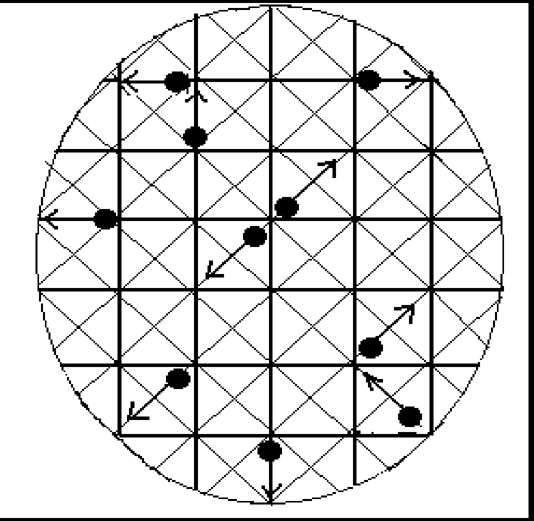
…or the flow of sheep!

Crash course on Hydrodynamics

Solving full NS equations may not be a great idea…

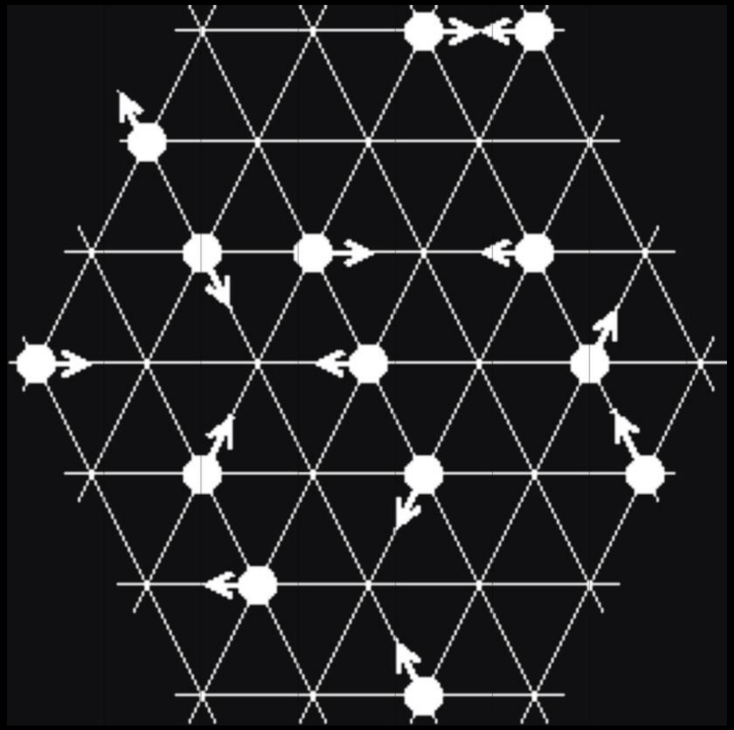


Be wise, discretize!



Marek Kac, 1914-1984

Lattice gas automata

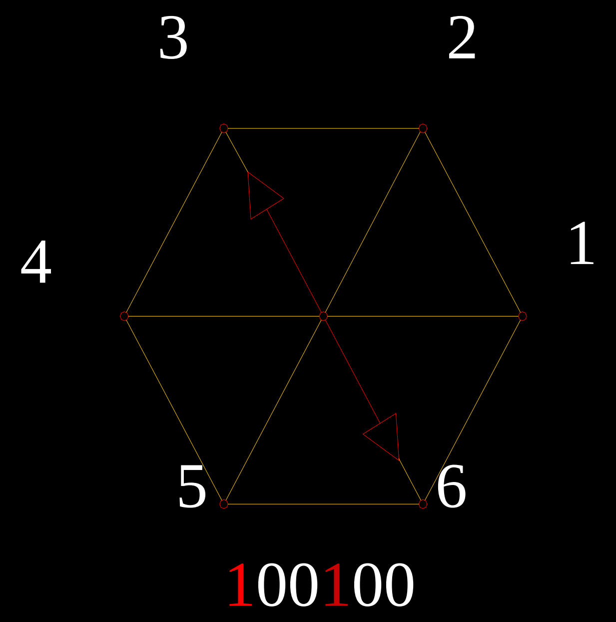


- streaming
- collisions

- positions restricted to lattice sites
- discrete velocities
- no two particles with the same velocity allowed at one site

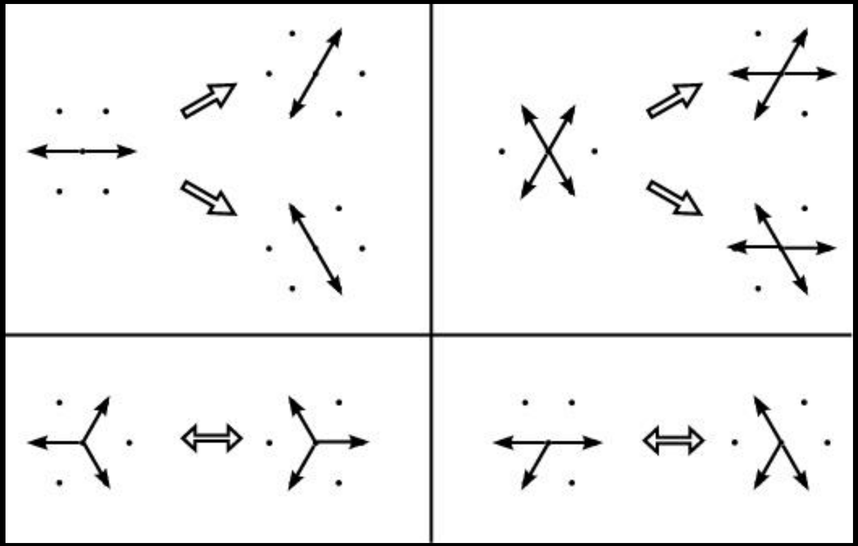
Boolean representation

$n_i = 0,1$ particle absence/presence



Collisions

Collision rules

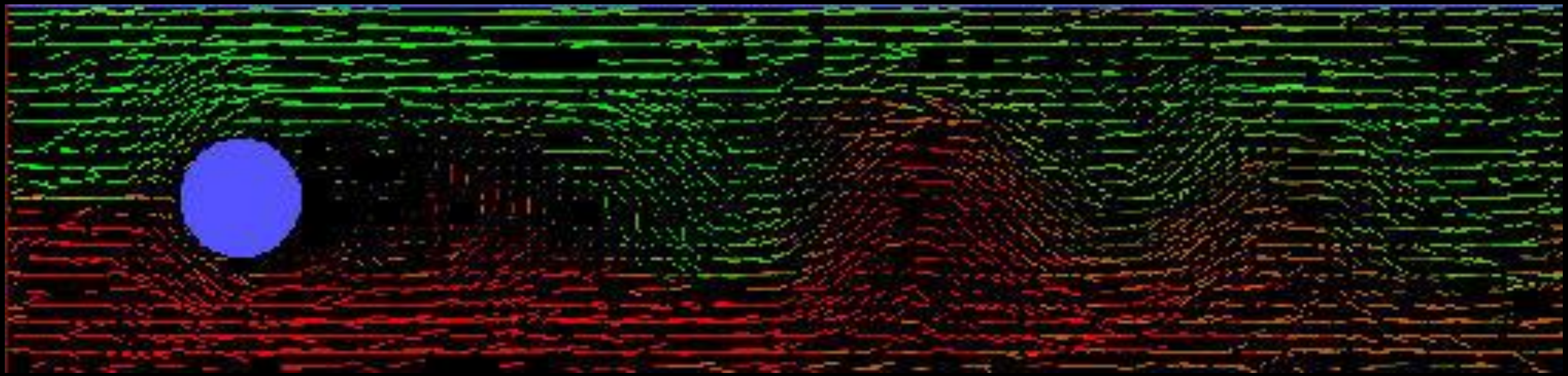


Binary representation

Input State	Output State
001001	010010 100100
010101	101010
001011	100110
011011	110110 101101

Very simple to implement numerically – **no floating point operations!**

Flow around a cylinder



Pros and cons

Pros:

- extremely simple to program,
- fast,
- exact, no round-off errors,
- inherently stable.

Cons:

- noisy,
- viscosity set by collision table (cannot be tuned).

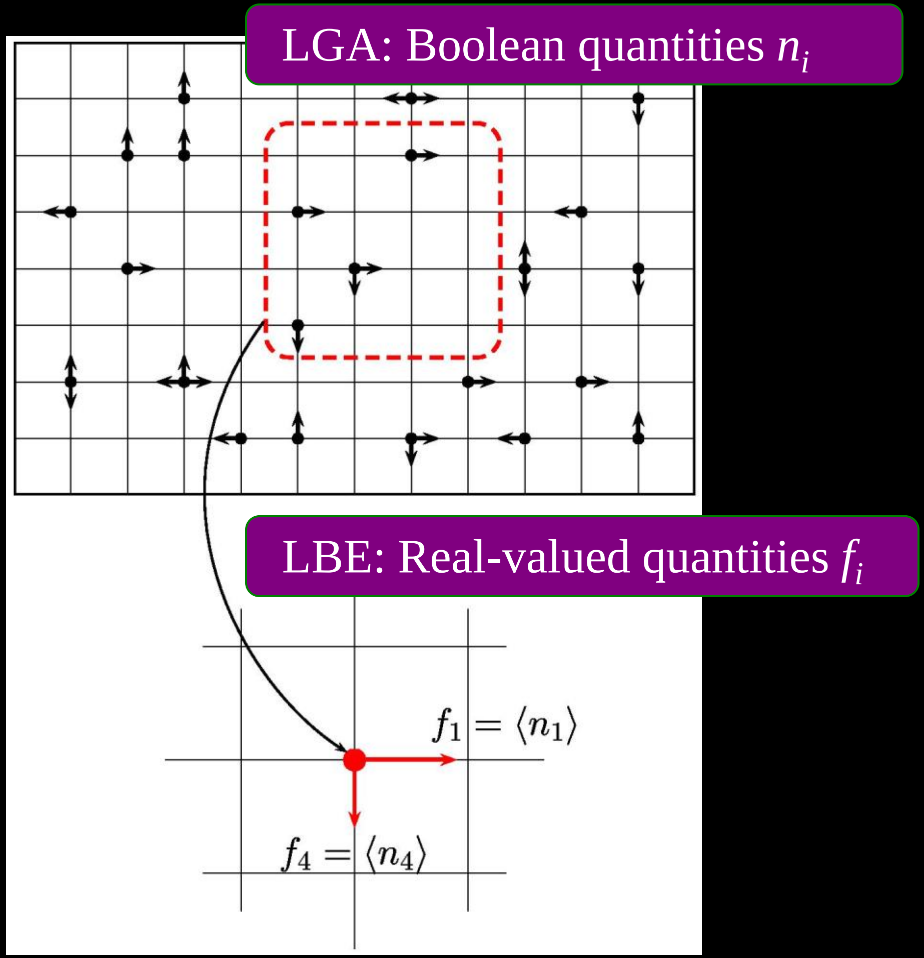
From LGA to LBE

One lattice node represents particle *densities*: discrete dynamics are replaced by a smooth flow.

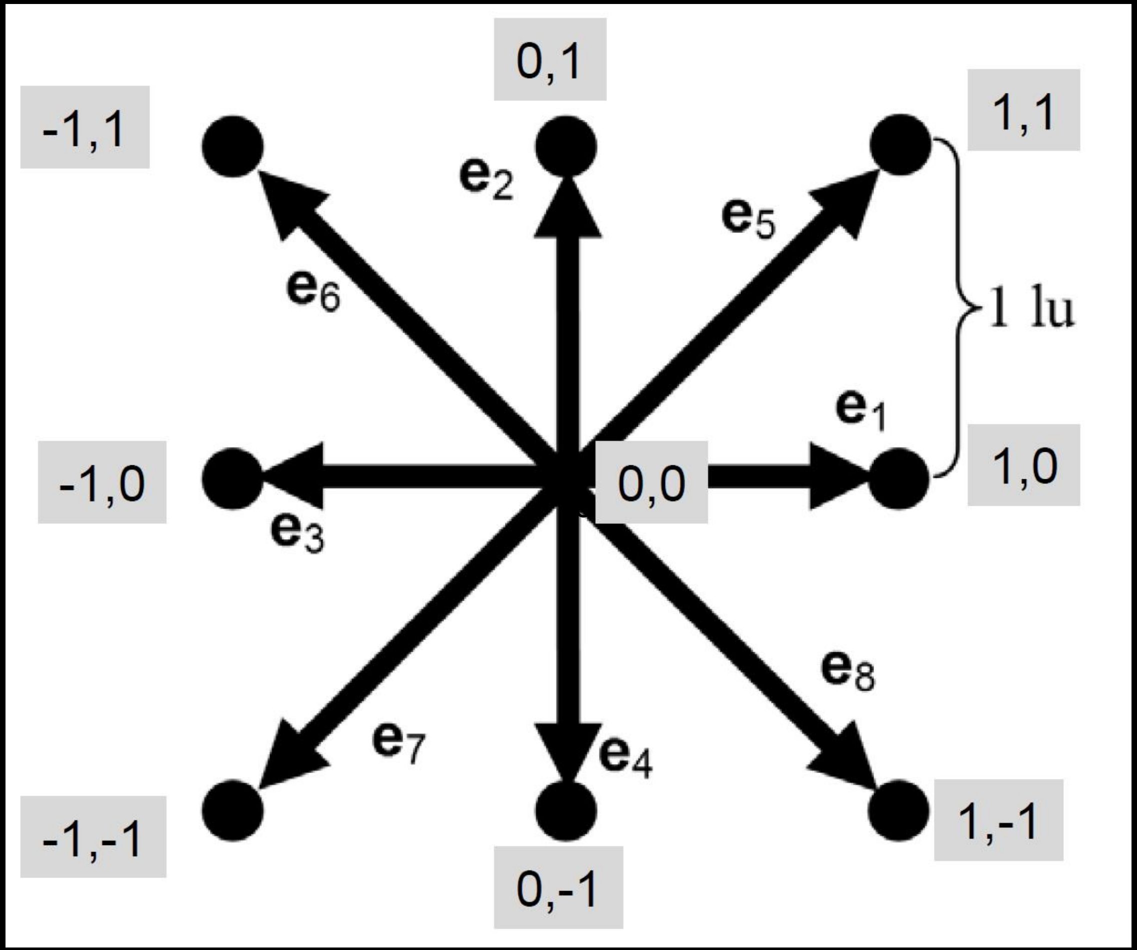
Less averaging needed, increased performance.

$$n_i \rightarrow f_i = \langle n_i \rangle$$

continuous population density, f_i



Discrete set of velocities



e = [[0, 0], [1, 0], [0, 1], [-1, 0], [0, -1], [1, 1], [-1, 1], [-1, -1], [1, -1]]

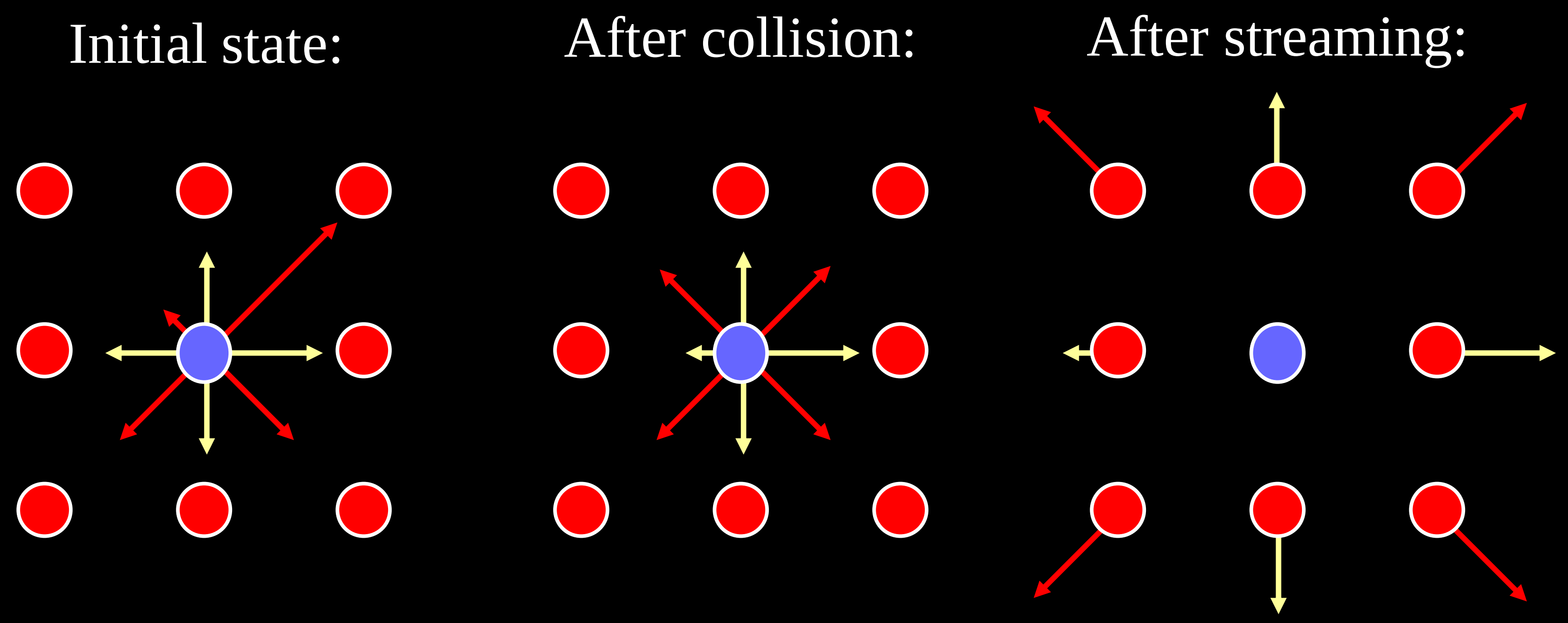
Hydrodynamic fields are moments of the distribution function f(**r**,t):

$$\rho(\mathbf{r}, t) = \sum_i f_i(\mathbf{r}, t)$$ Mass

$$\rho(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t) = \sum_i f_i(\mathbf{r}, t)\, \boldsymbol{e}_i$$ Momentum

where $\mathbf{e}_i$ are the discrete velocities in the model

Lattice-Boltzmann model:



Evolution equation

$$\boxed{f_i(\mathbf{r} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{r}, t) - [f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)]/\tau}$$

relaxation-time form of the collision operator

$f_i^{eq}(\mathbf{r}, t)$ - equilibrium distribution

Equilibrium distribution is an expansion of the local Maxwell distribution.

Equilibrium distribution

- start from the Maxwell distribution $$f^{eq} = \frac{\rho}{2\pi RT} \exp\left(\frac{-(\mathbf{e}-\mathbf{u})^2}{2RT}\right)$$

- normalize the velocities by $\sqrt{3RT}$: $$f^{eq} = \frac{\rho}{2\pi/3} \exp\left(-\frac{3}{2}(\mathbf{e}-\mathbf{u})^2\right)$$

- expand in u up to $O(u^2)$:

$$f^{eq} = \frac{\rho}{2\pi/3} \exp\left(-\frac{3}{2}\mathrm{e}^2\right)\left[1 + 3(\mathbf{e}\cdot\mathbf{u}) + \frac{9}{2}(\mathbf{e}\cdot\mathbf{u})^2 - \frac{3}{2}\mathrm{u}^2\right]$$

- for discrete set of velocities e_i the corresponding distribution functions read

$$f_i^{eq} = W_i \rho\left[1 + 3(\mathbf{e}_i\cdot\mathbf{u}) + \frac{9}{2}(\mathbf{e}_i\cdot\mathbf{u})^2 - \frac{3}{2}\mathrm{u}^2\right]$$

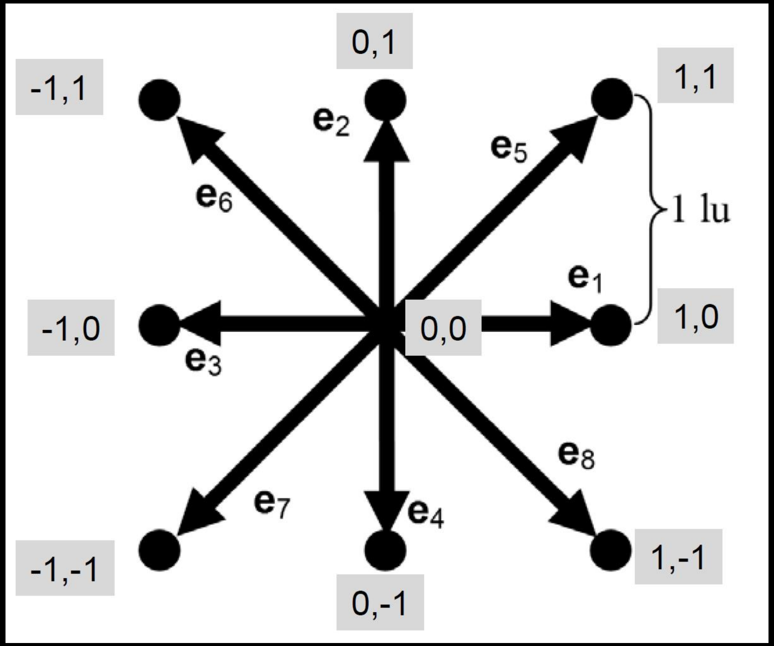
Equilibrium distribution (2)

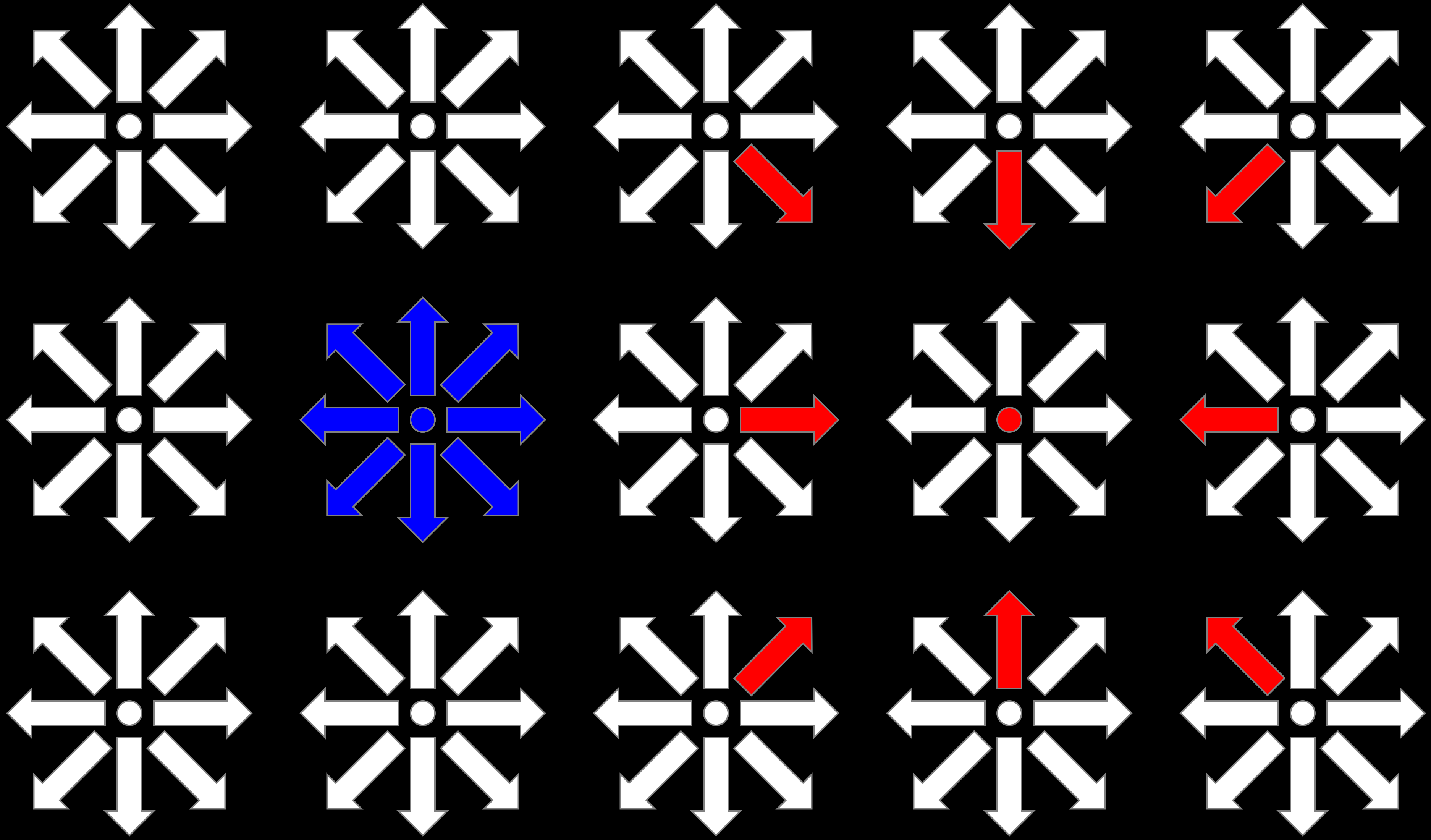
The weights W_i are then determined from the isotropy conditions and the moment conditions:

$$\rho = \sum_i f_i^{eq}, \qquad \rho\mathbf{u} = \sum_i f_i^{eq}\, e_i$$

For the 2D square lattice with nine velocities one gets:

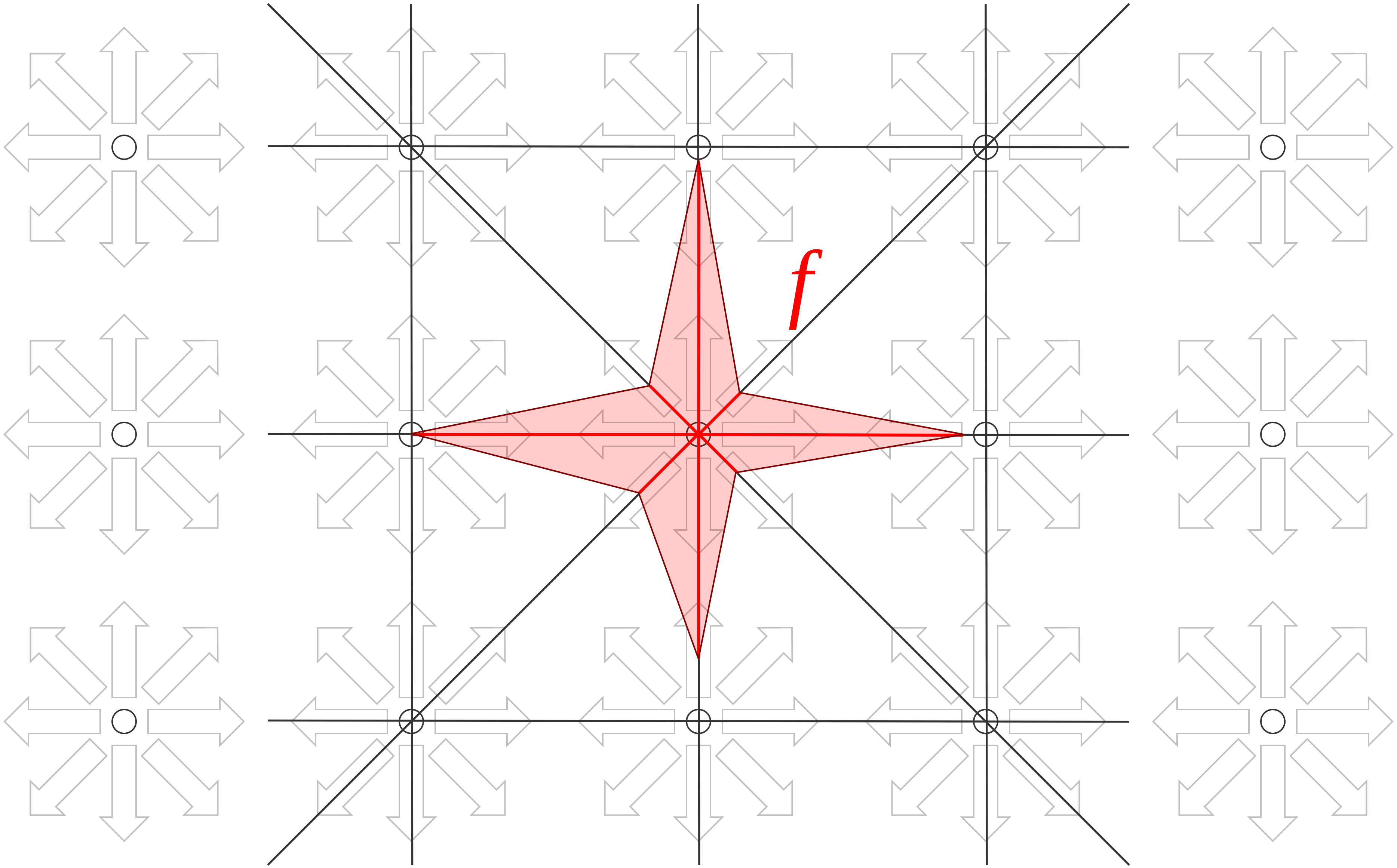
$$W_0 = 4/9$$
$$W_1 = W_2 = W_3 = W_4 = 1/9$$
$$W_5 = W_6 = W_7 = W_8 = 1/36$$





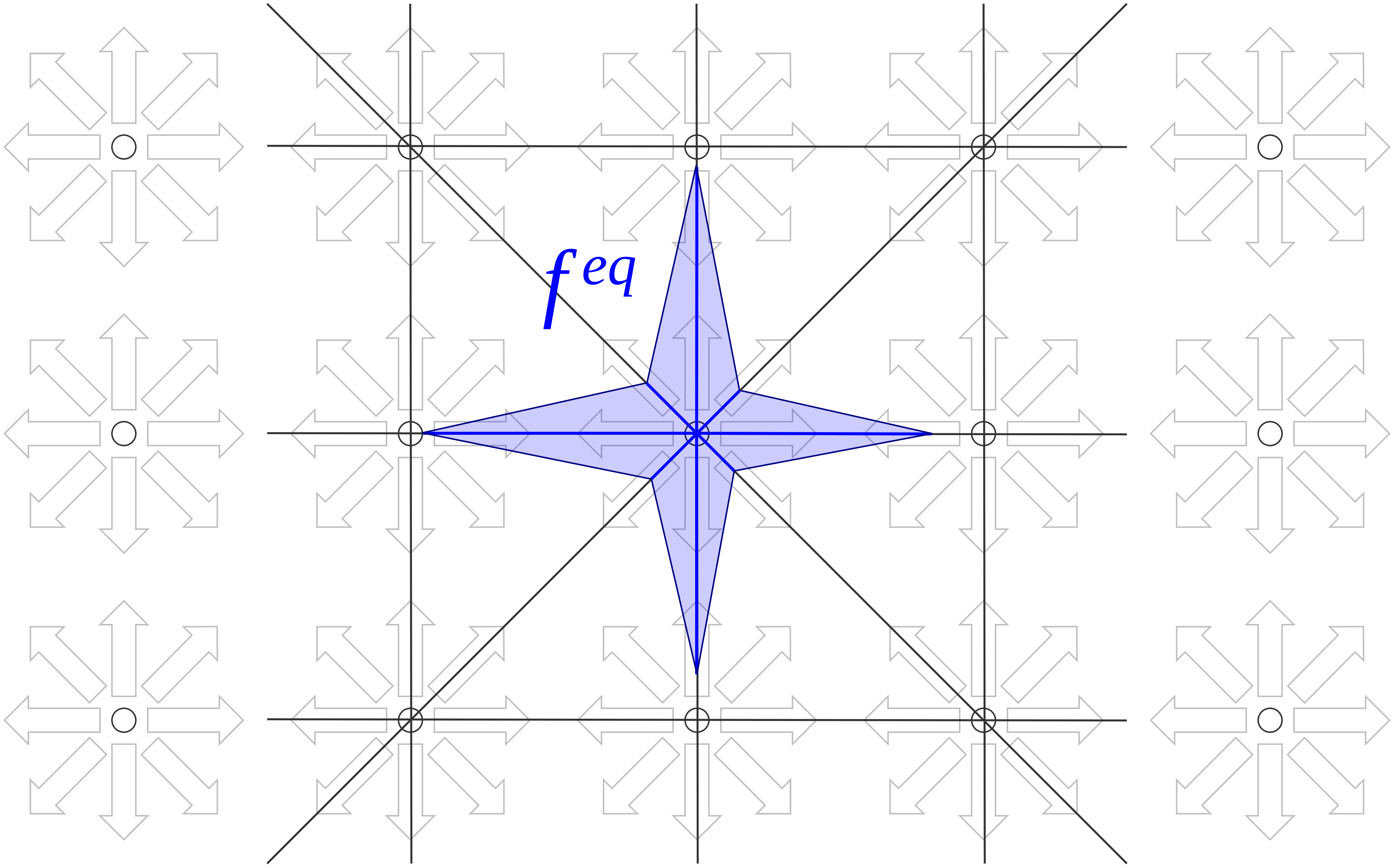
animation by D.Thorne and M.Sukop
(FIU, Miami)

streaming step



animation by D.Thorne and M.Sukop
(FIU, Miami)

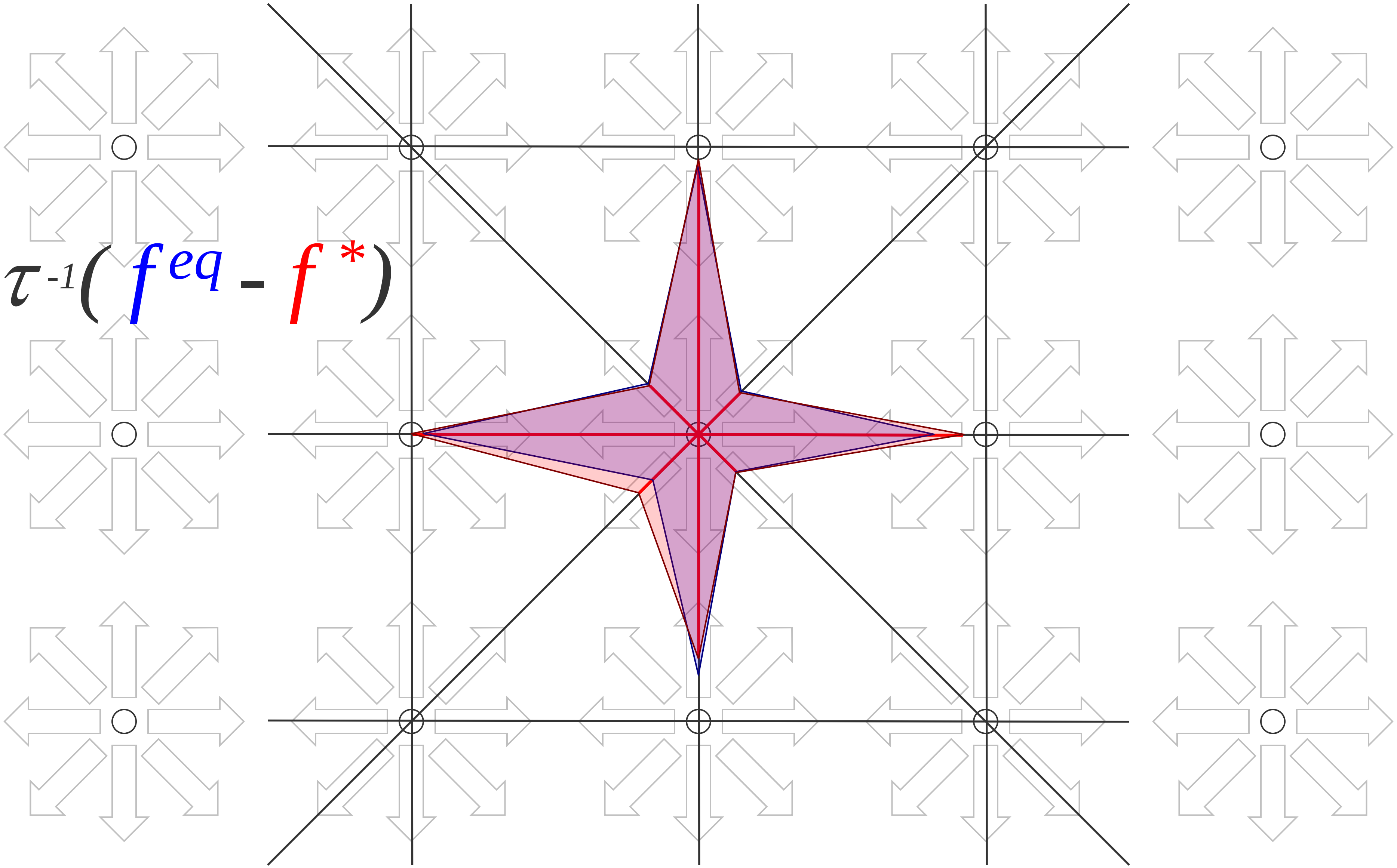
collision step



animation by D.Thorne and M.Sukop
(FIU, Miami)

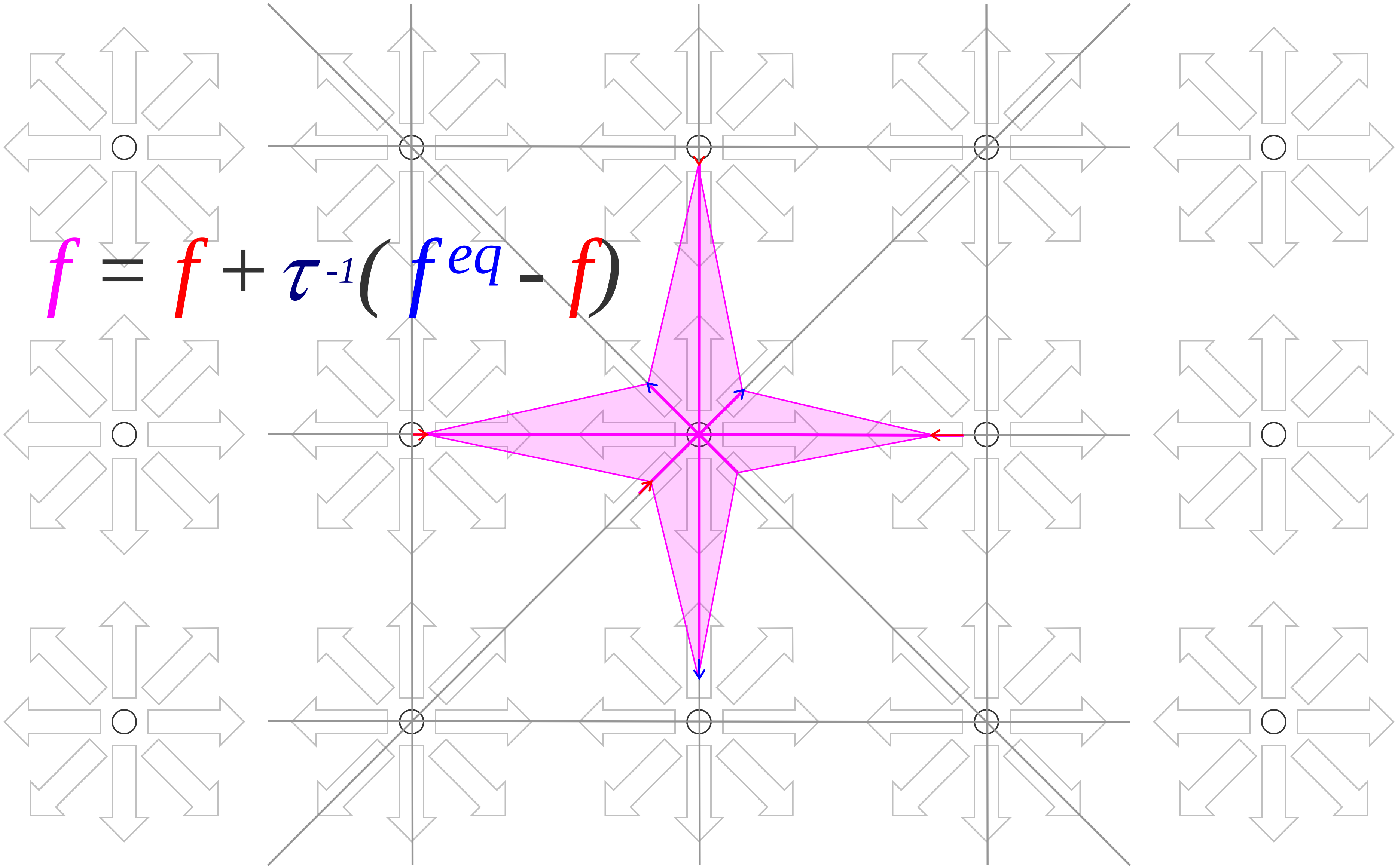
collision step

$\tau^{-1}(f^{eq} - f^{*})$



animation by D.Thorne and M.Sukop
(FIU, Miami)

collision step



animation by D.Thorne and M.Sukop
(FIU, Miami)

collision step

LBM to Navier-Stokes

- start from lattice Boltzmann equation

$$f_i(\mathbf{r} + \mathbf{c}_i\Delta t, t + \Delta t) - f_i(\mathbf{r}, t) = -[f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)]/\tau$$

- Taylor expand $f_i(\mathbf{r} + \mathbf{c}_i\Delta t, t + \Delta t)$ about ($\mathbf{r}$,t) to 2nd order in Δt

- write $f_i = f_i^{eq} + f_i^{neq}$ and note that $\rho = \sum_i f_i^{eq}$ and $\rho\mathbf{u} = \sum_i f_i^{eq}\mathbf{c}_i$

- in the incompressible limit you get the

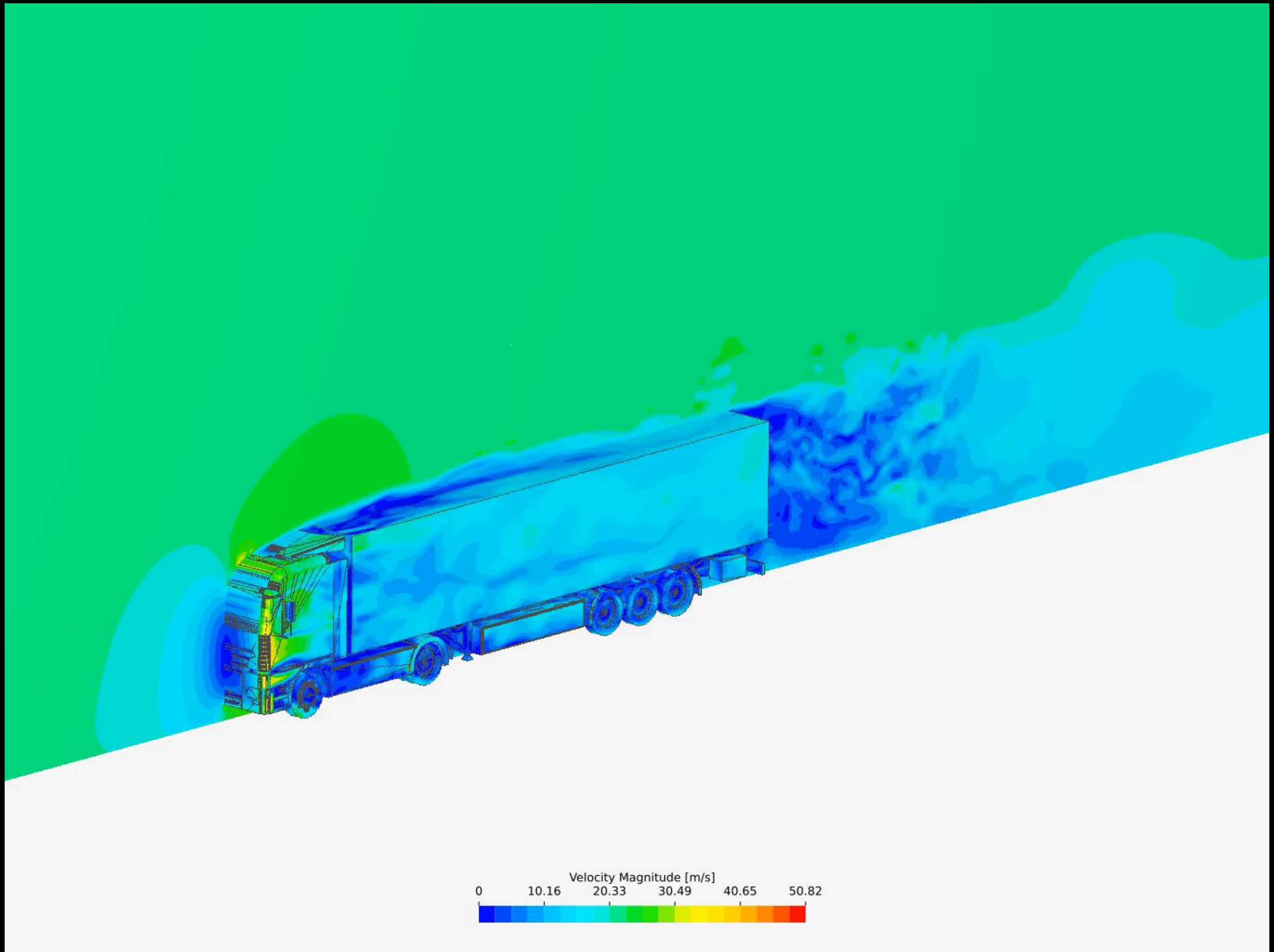
Navier Stokes equation

$$\boxed{\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u}}$$

with

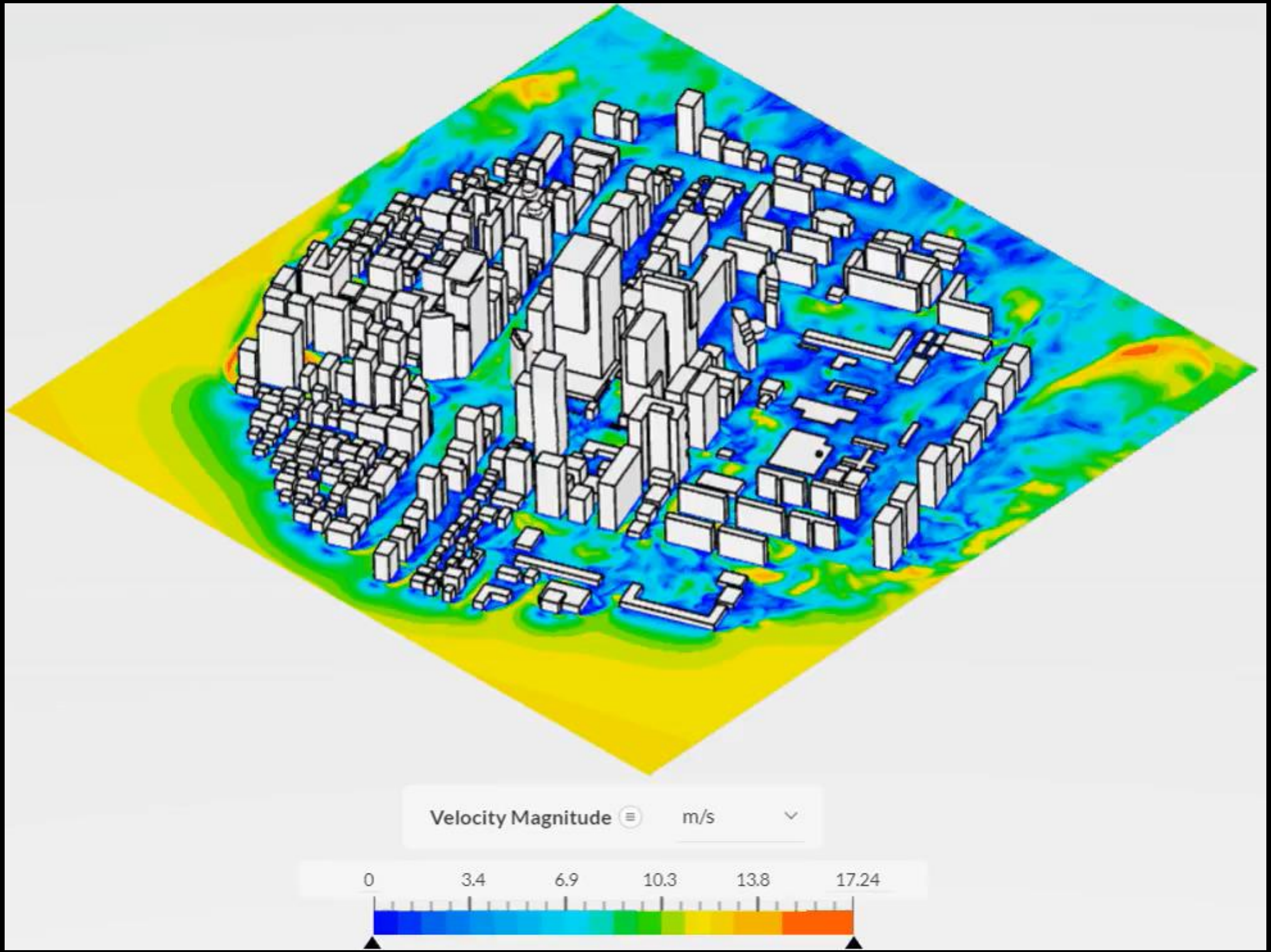
$$\nu = (\tau - \frac{1}{2})\frac{\Delta t}{3}$$

Examples (1)

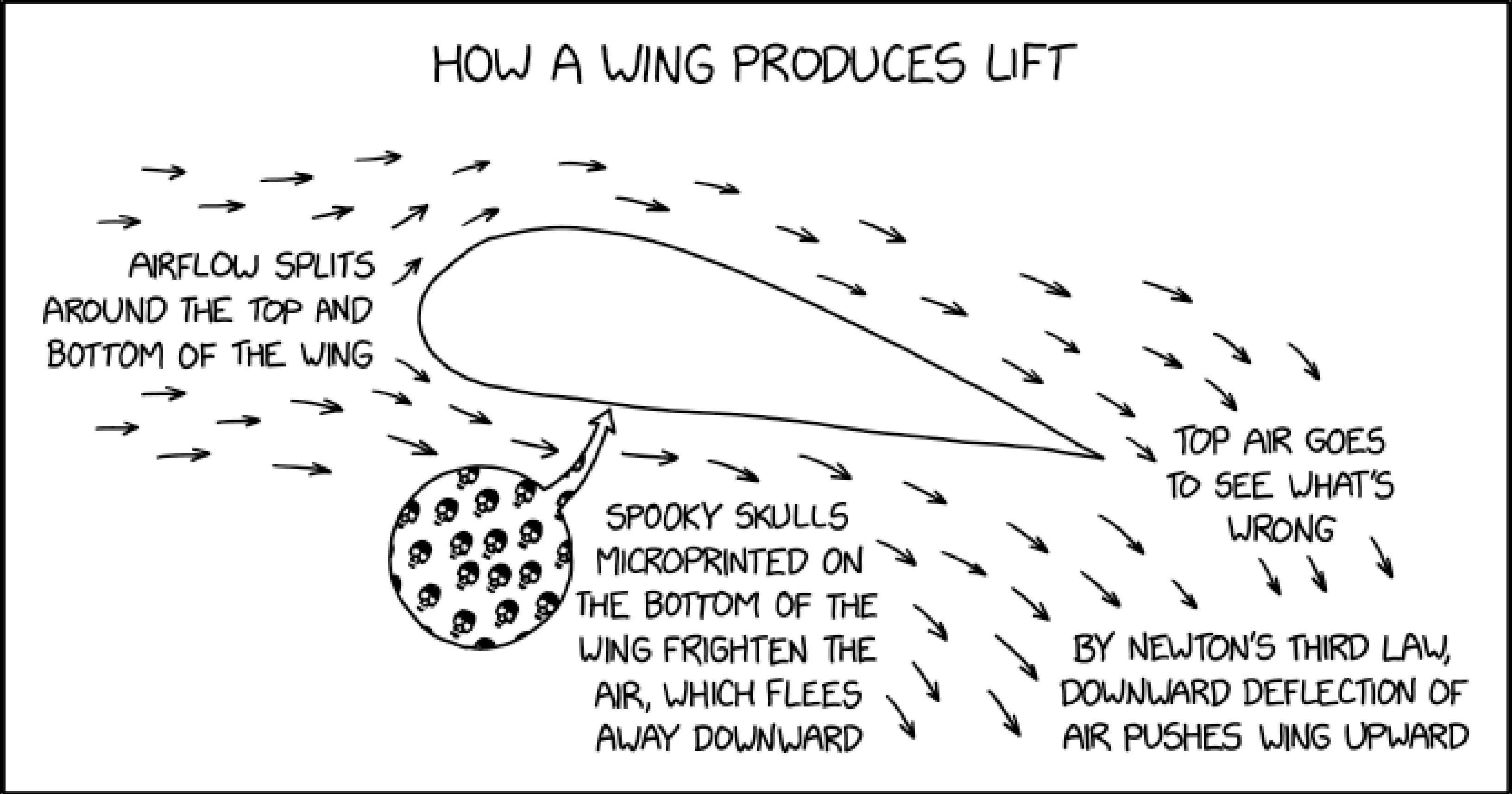


https://www.simscale.com

Examples (2)



https://www.simscale.com


HOW A WING PRODUCES LIFT
AIRFLOW SPLITS AROUND THE TOP AND BOTTOM OF THE WING
SPOOKY SKULLS MICROPRINTED ON THE BOTTOM OF THE WING FRIGHTEN THE AIR, WHICH FLEES AWAY DOWNWARD
TOP AIR GOES TO SEE WHAT'S WRONG
BY NEWTON'S THIRD LAW, DOWNWARD DEFLECTION OF AIR PUSHES WING UPWARD