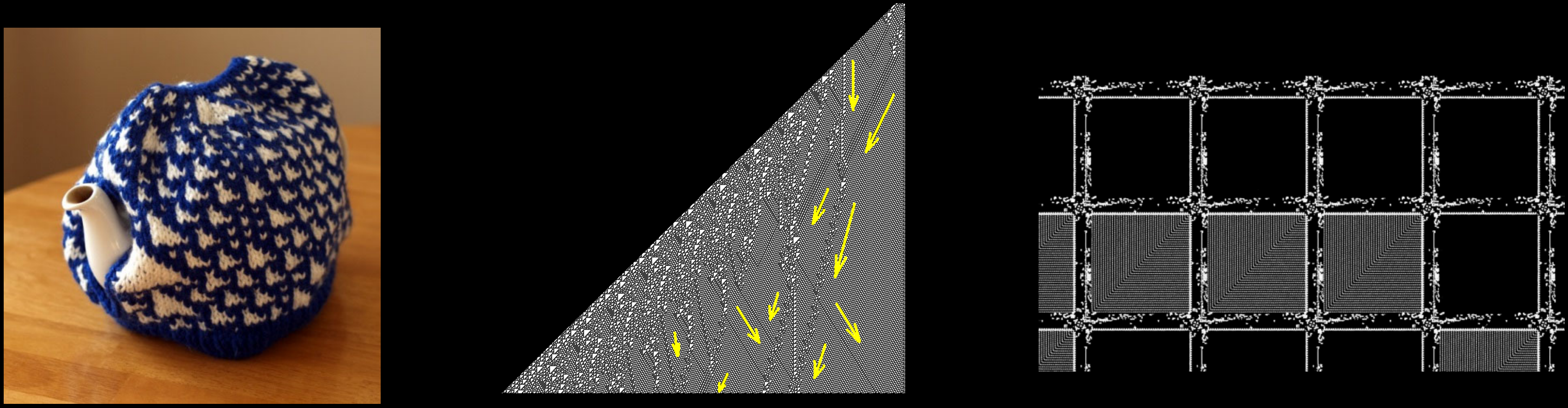
Computer modeling of physical phenomena

Lecture X : Lattice Gases & Lattice Boltzmann Method

Cellular automata

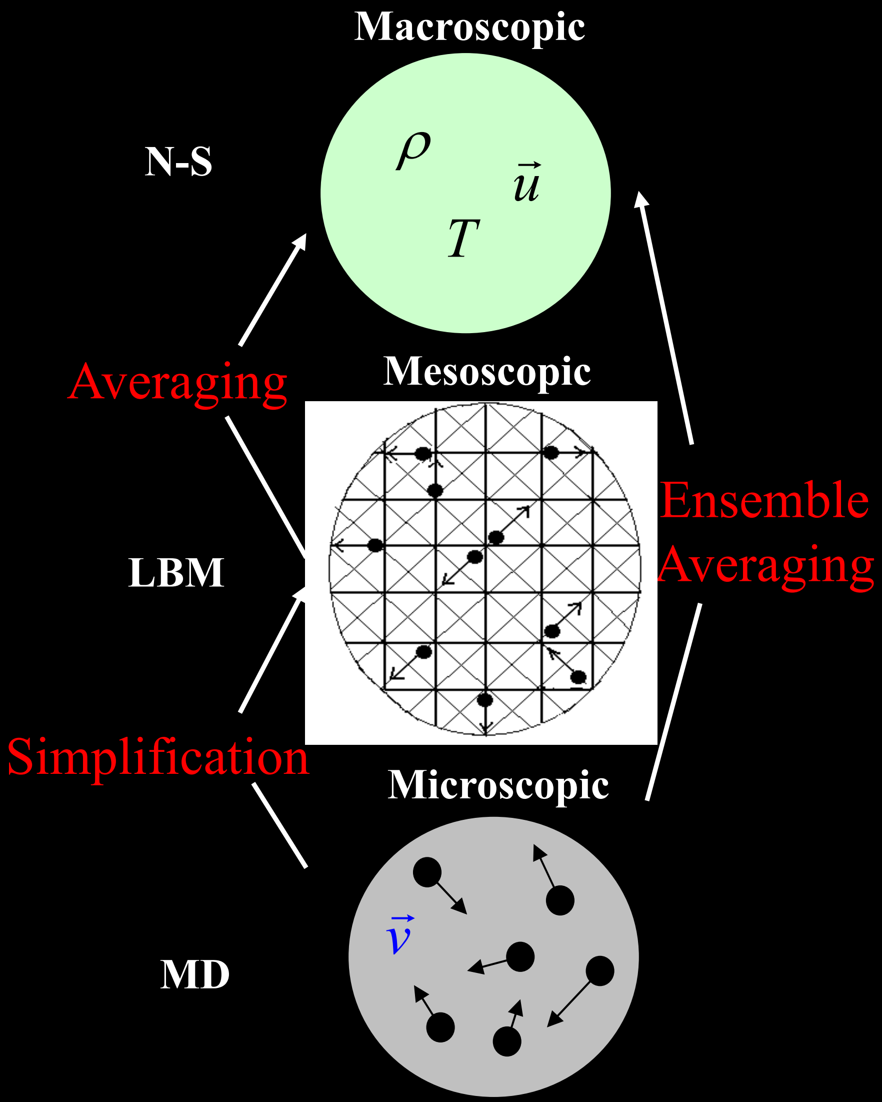


It’s all very nice but....

What it has to do with physics.?

Lattice Gases and Lattice Boltzmann Method

Mesoscopic approach



Macroscopic

N-S

ρ $\vec{u}$ T

Averaging

Mesoscopic

LBM

Ensemble Averaging

Simplification

Microscopic

MD

$\vec{v}$

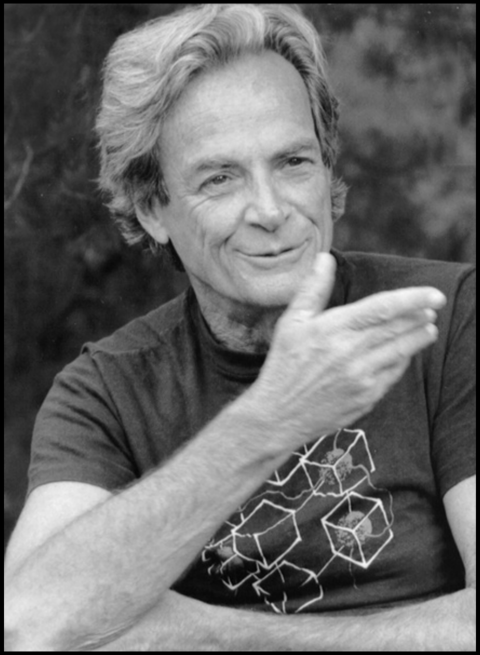
Lattice-particle methods

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

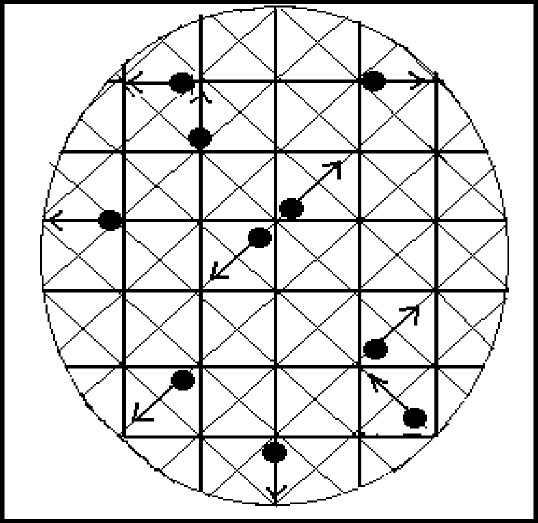
Feynman on lattice automata

„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 or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids."



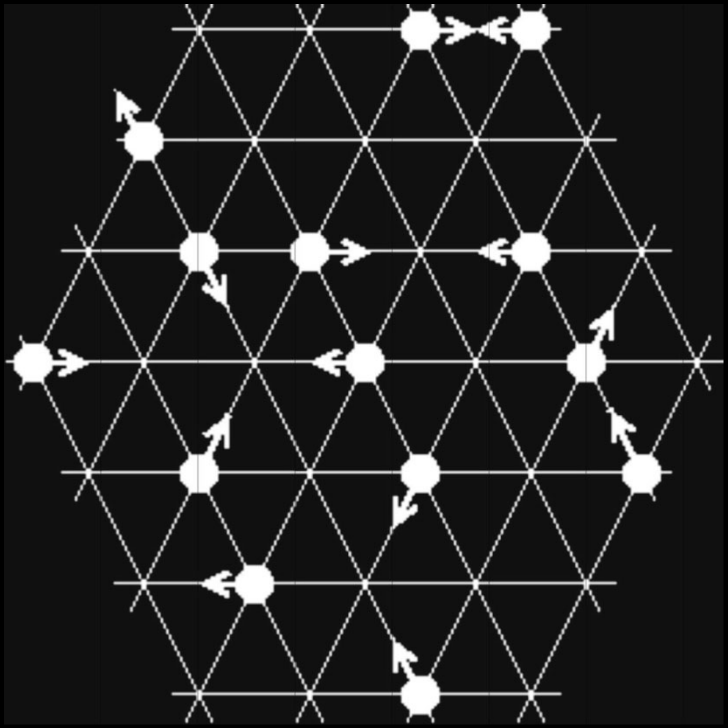
W. Daniel Hillis. Richard Feynman and the Connection Machine. Physics Today, 42:78 1989.

Be wise, discretize!



Marek Kac, 1914-1984

Lattice gas automata

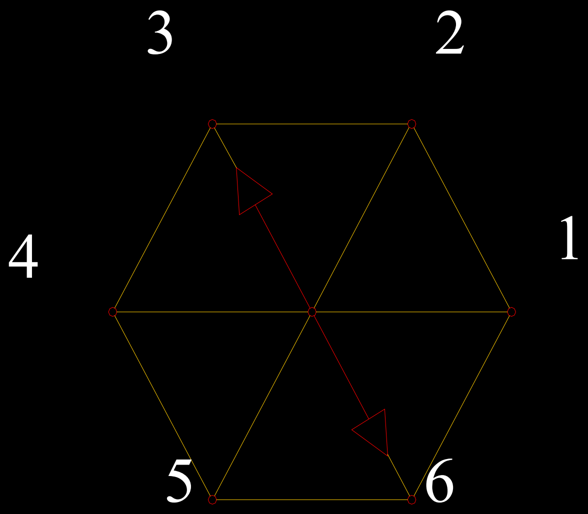


- streaming
- collisions

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

Boolean representation

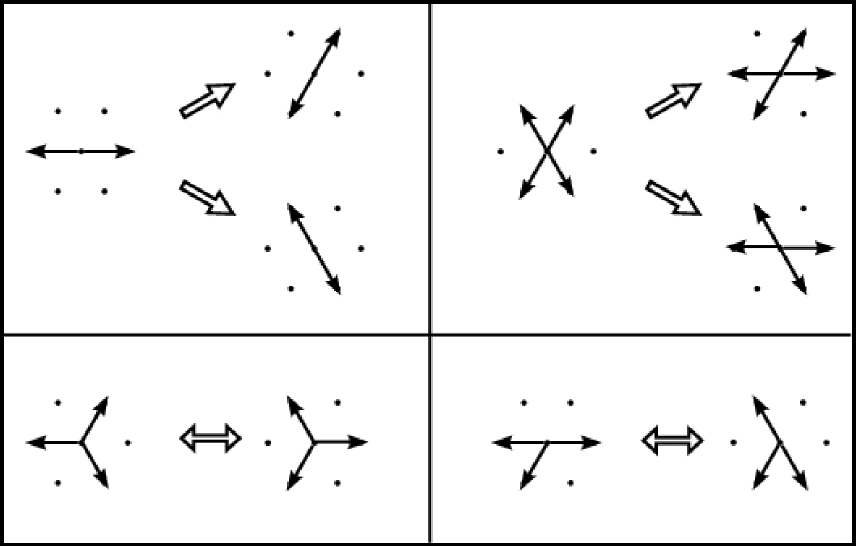
$n_i=0,1$ particle absence/presence



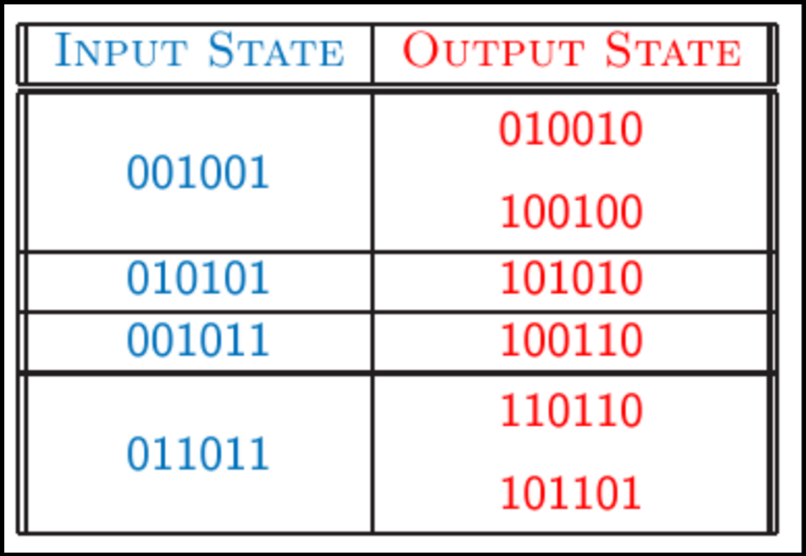
100100

Collisions

Collision rules



Binary representation

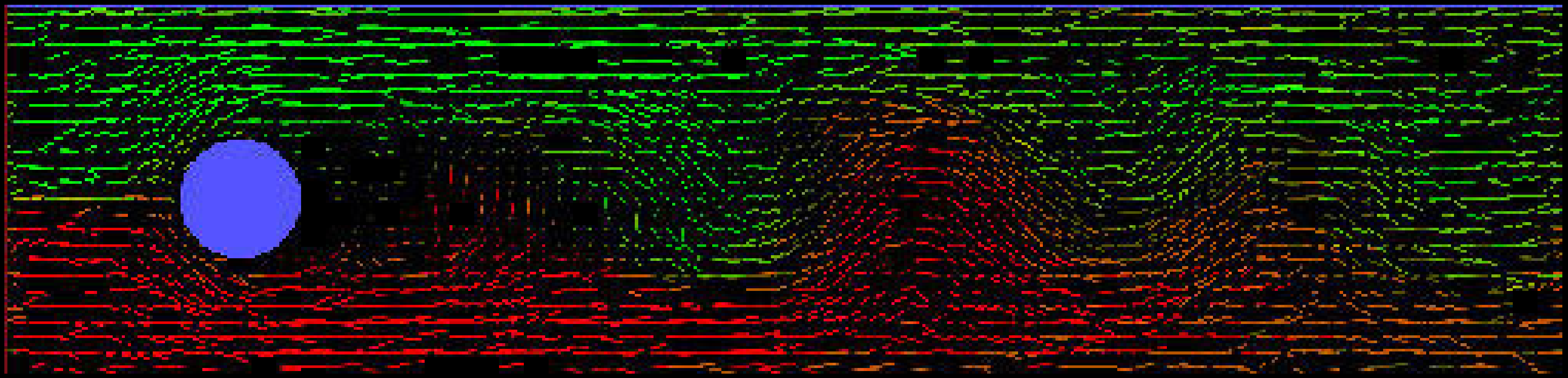


INPUT STATE	OUTPUT STATE
001001	010010 100100
010101	101010
001011	100110
011011	110110 101101

Very simple to implement numerically, especially on dedicated computers

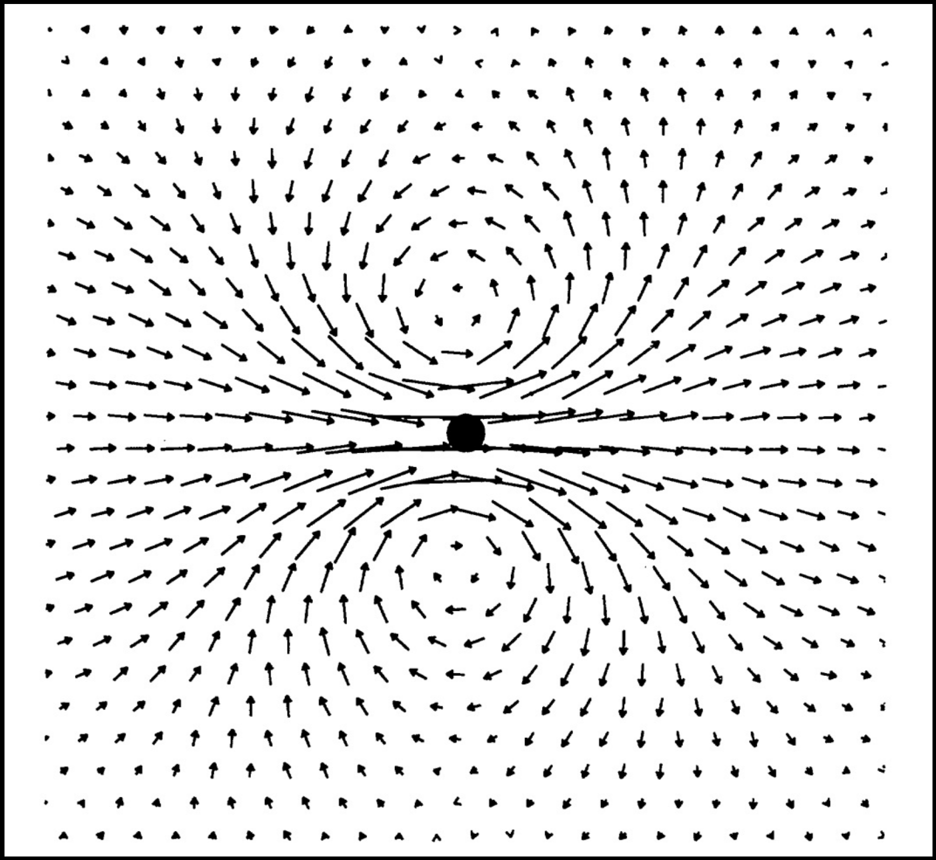
no floating point operations, roundoff errors etc!

Von Karman street



(Sauro Succi)

Moving particles



(Van der Hoef, Frenkel & Ladd, PRL 1991)

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)

$$\eta = 1.23\, m\, l \,/\, \Delta t$$

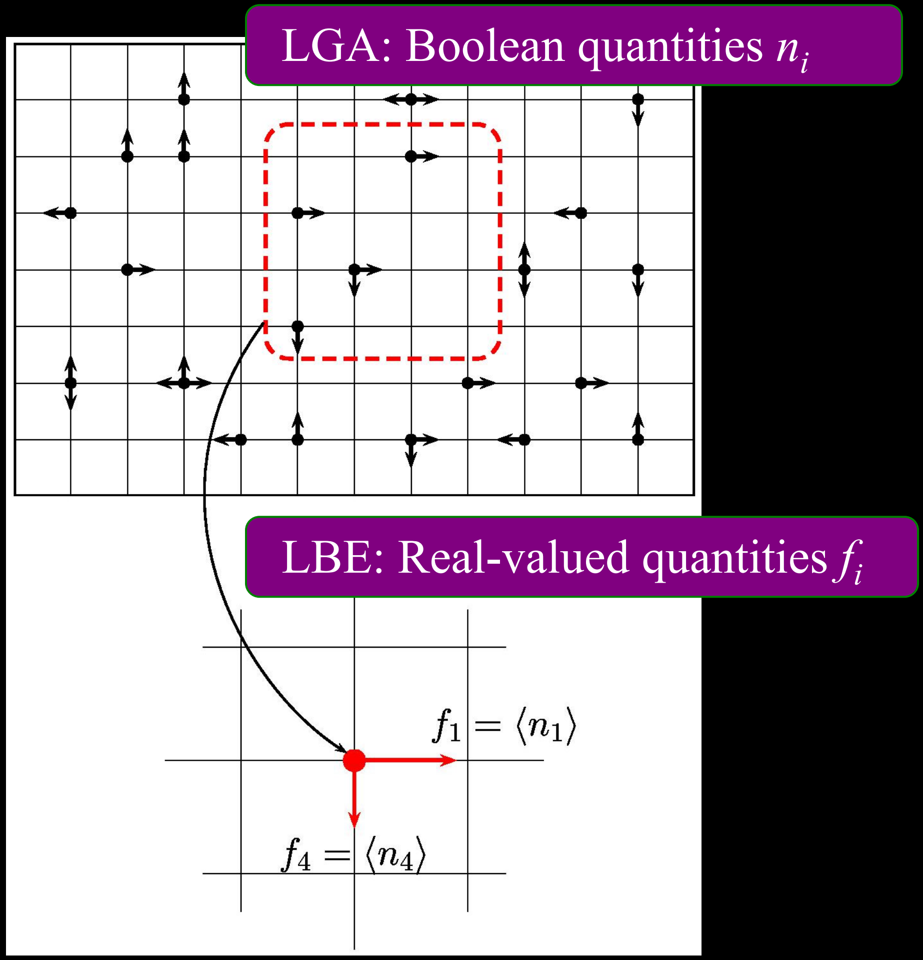
From LGA to LBE

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

Less averaging needed, increased performance.

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

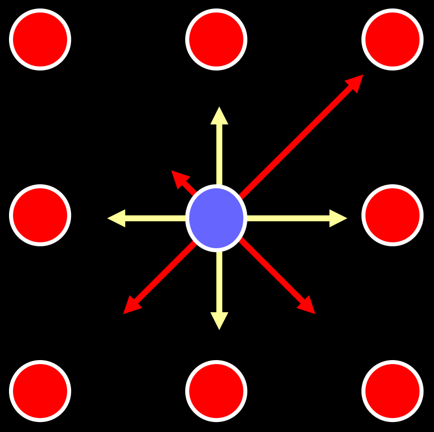
Continuous population density, f_i



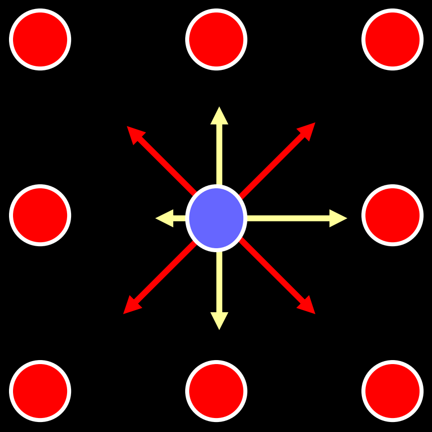
LGA: Boolean quantities n_i

LBE: Real-valued quantities f_i

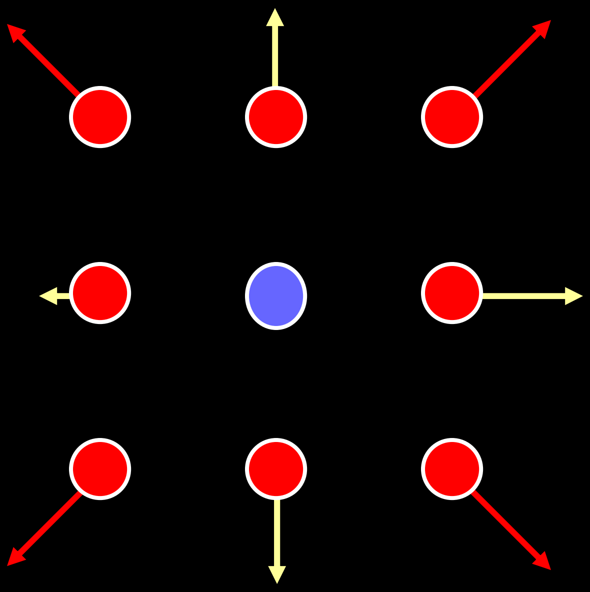
Lattice-Boltzmann model:



Initial State:

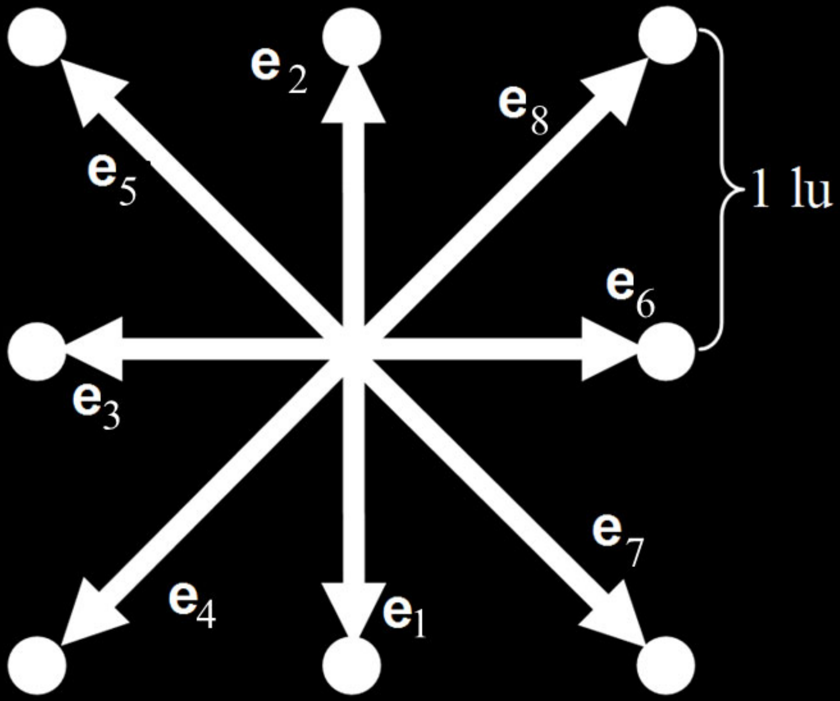


Post-Collision:



Propagation

Discrete set of velocities



c=[[0, 0],[0, -1],[0, 1],[-1, 0],[-1, -1],[-1, 1],[1, 0],[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

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

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

Evolution equation

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

single relaxation-time form of the collision operator (analogous to BGK model in kinetic theory)

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

Equilibrium distribution is a small *u* expansion of the local Maxwell distribution →

Equilibrium distribution

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

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

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

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

- for discrete set of velocities c_i (i=1,…,M) the corresponding distribution functions read

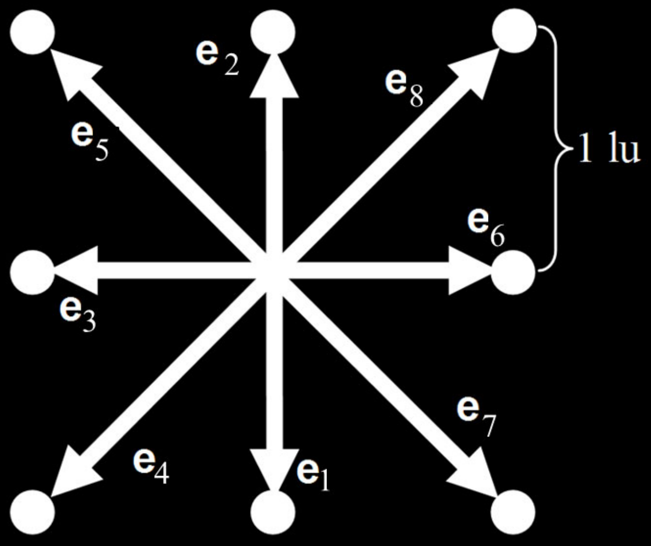
$$f_i^{eq} = W_i\rho[1+3(\mathbf{c}_i\cdot\mathbf{u})+\frac{9}{2}(\mathbf{c}_i\cdot\mathbf{u})^2-\frac{3}{2}u^2]$$

Equilibrium distribution (2)

the weights W_i are then determined from the isotropy conditions and the moment conditions: $\rho = \sum_i f_i^{eq}, \qquad \rho \mathbf{u} = \sum_i f_i^{eq} \mathbf{c}_i$

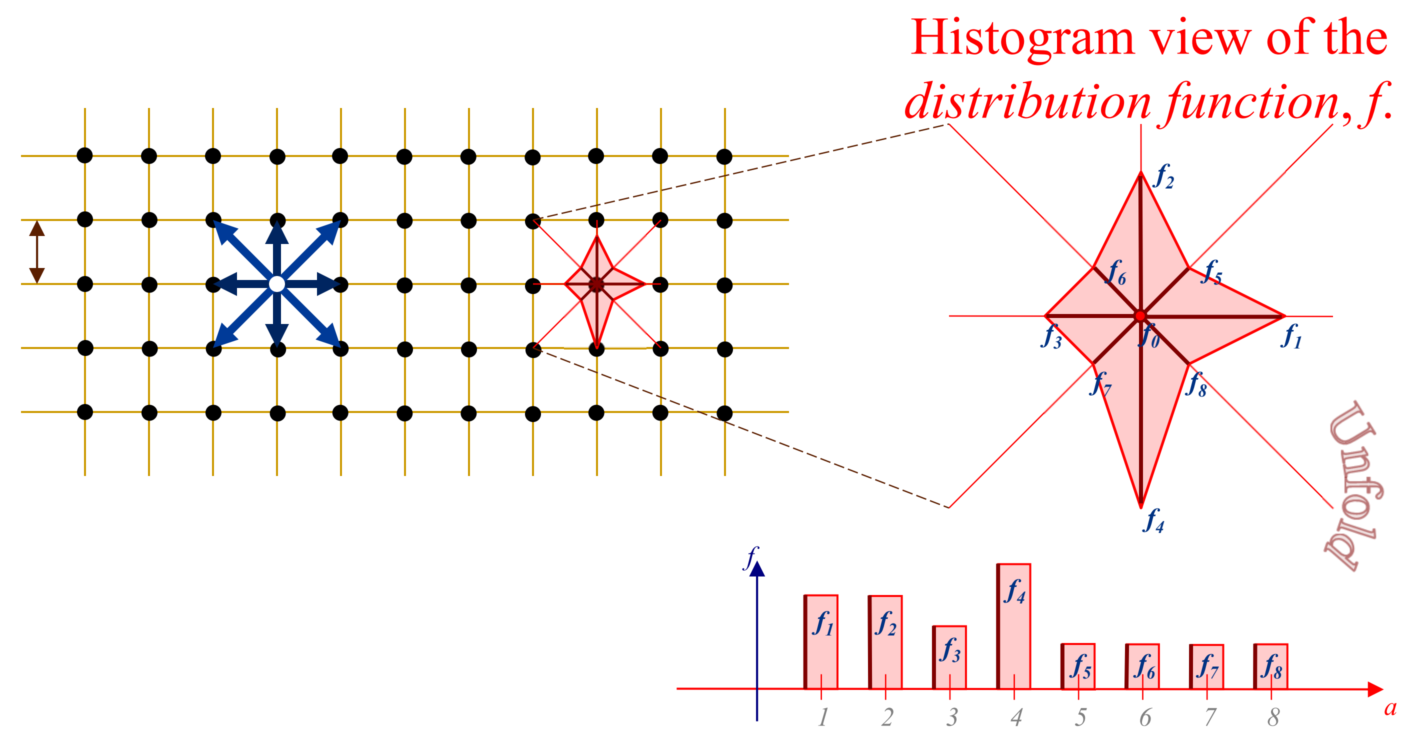
for the 2d square lattice with nine velocities one gets:

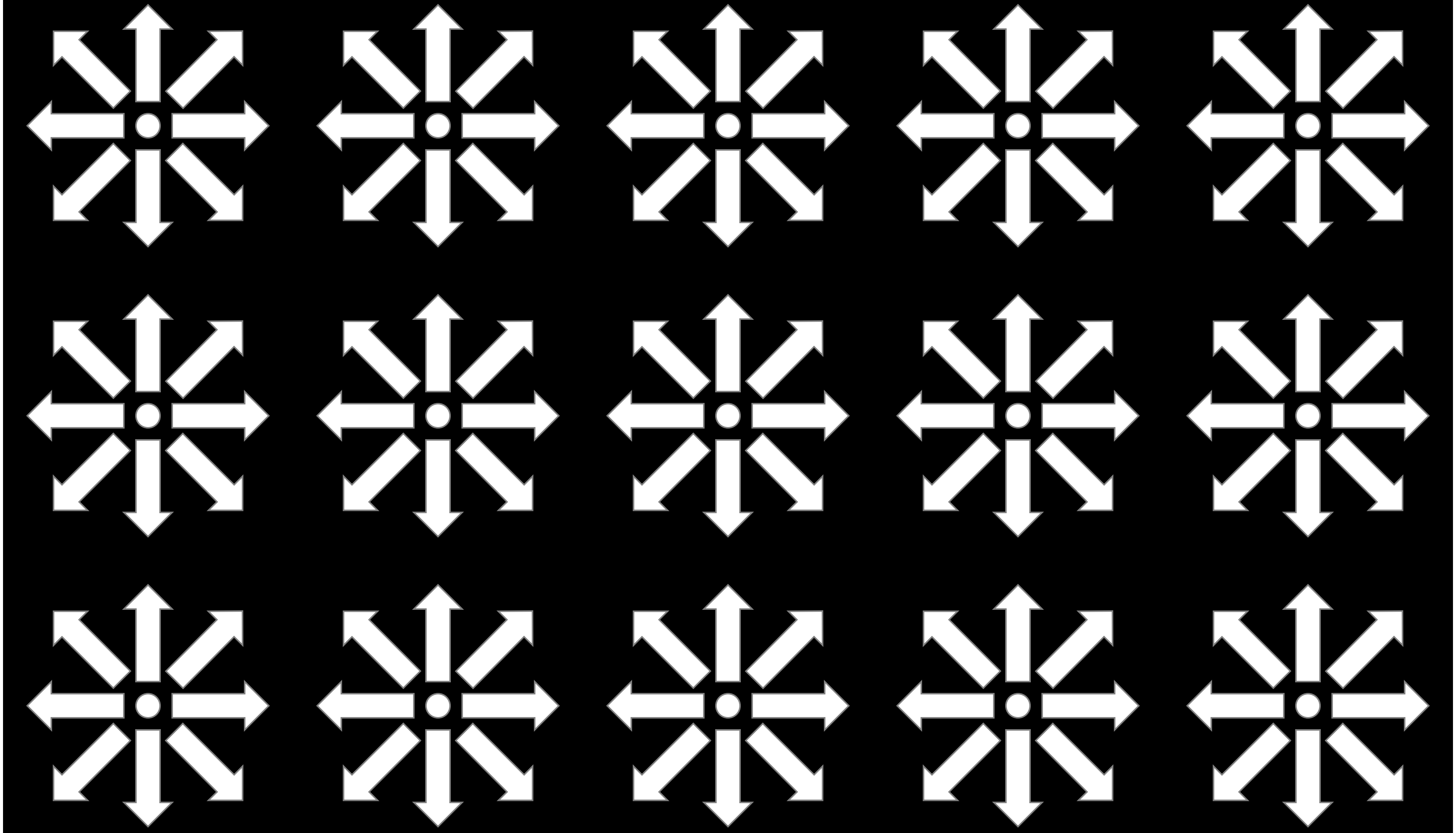
$$W_0 = 4/9$$
$$W_1 = W_2 = W_3 = W_6 = 1/9$$
$$W_4 = W_5 = W_7 = W_8 = 1/36$$



Illustration

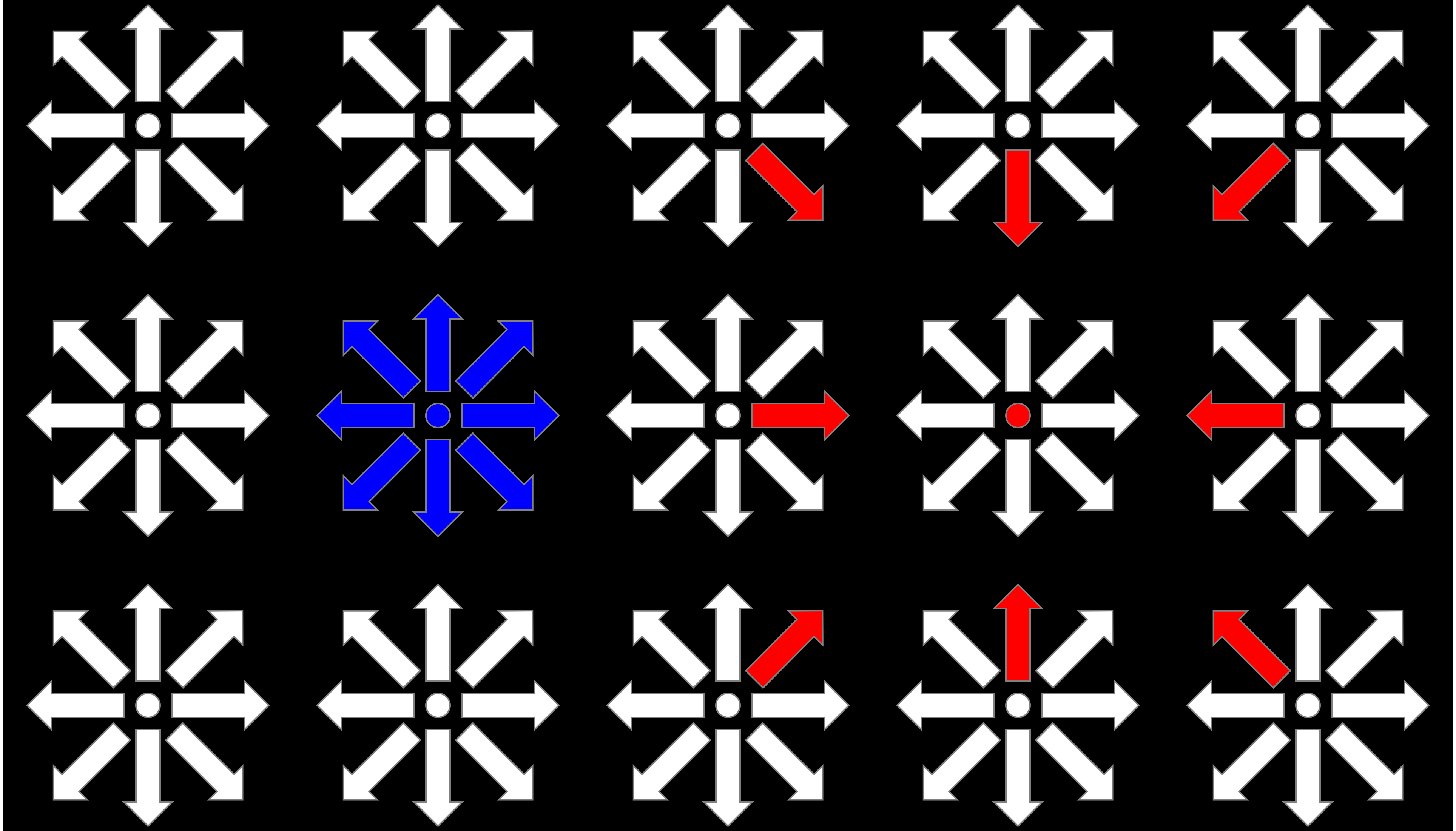
animation of streaming and collision steps in Lattice Boltzmann by D.Thorne and M.Sukop (FIU, Miami)


Histogram view of the *distribution function*, *f*.



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

streaming step



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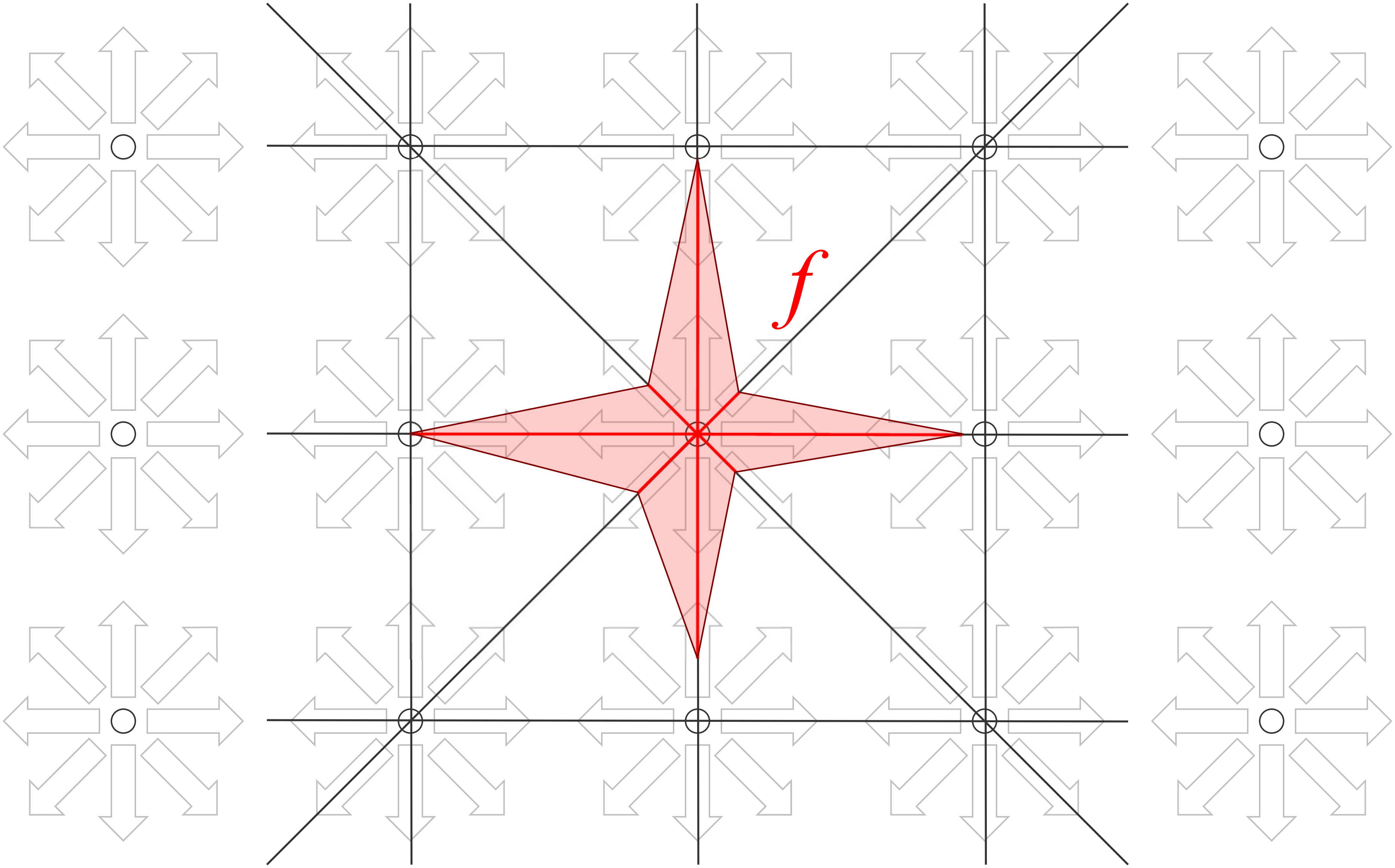
streaming step



animation by D.Thorne and M.Sukop
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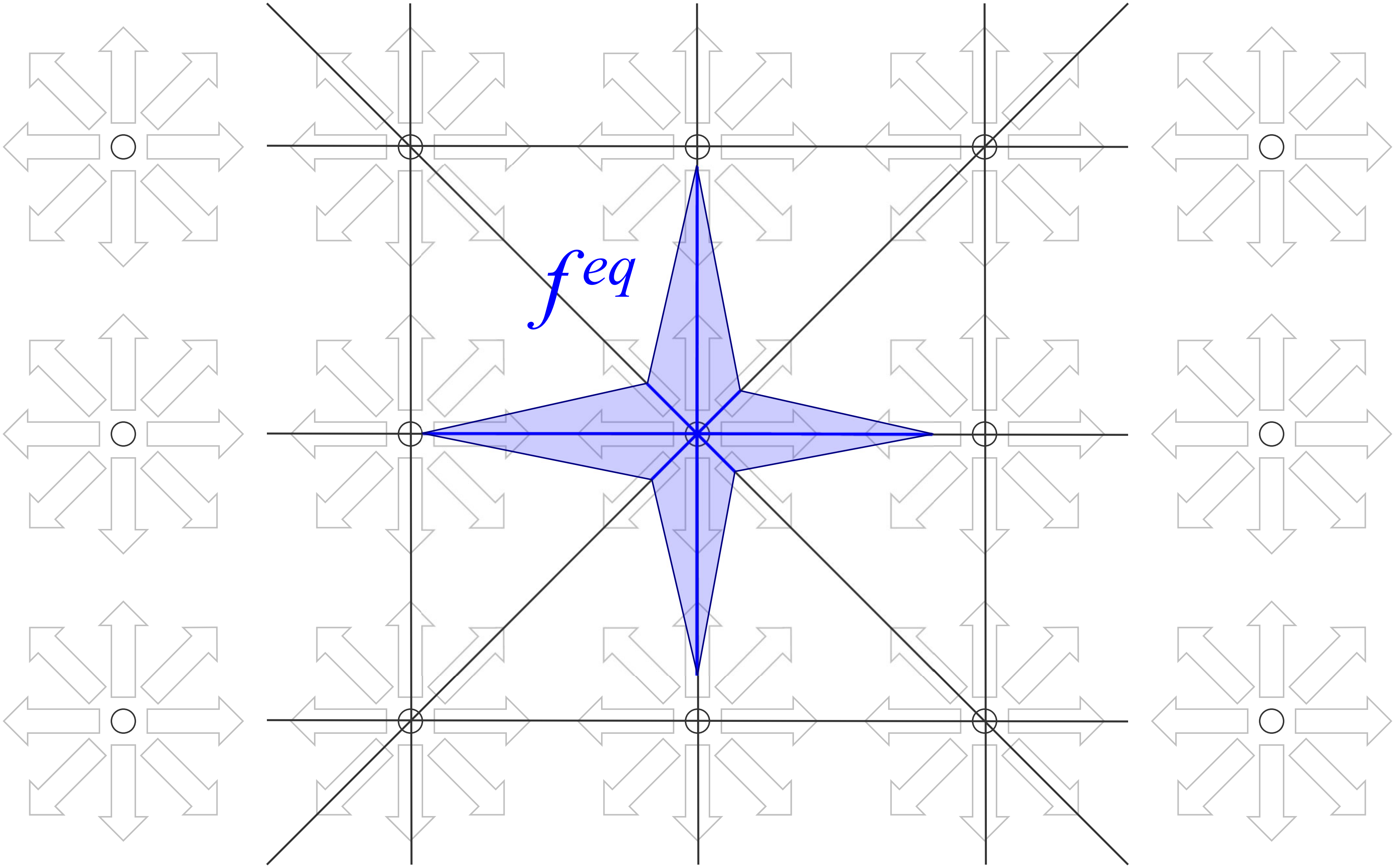
collision step



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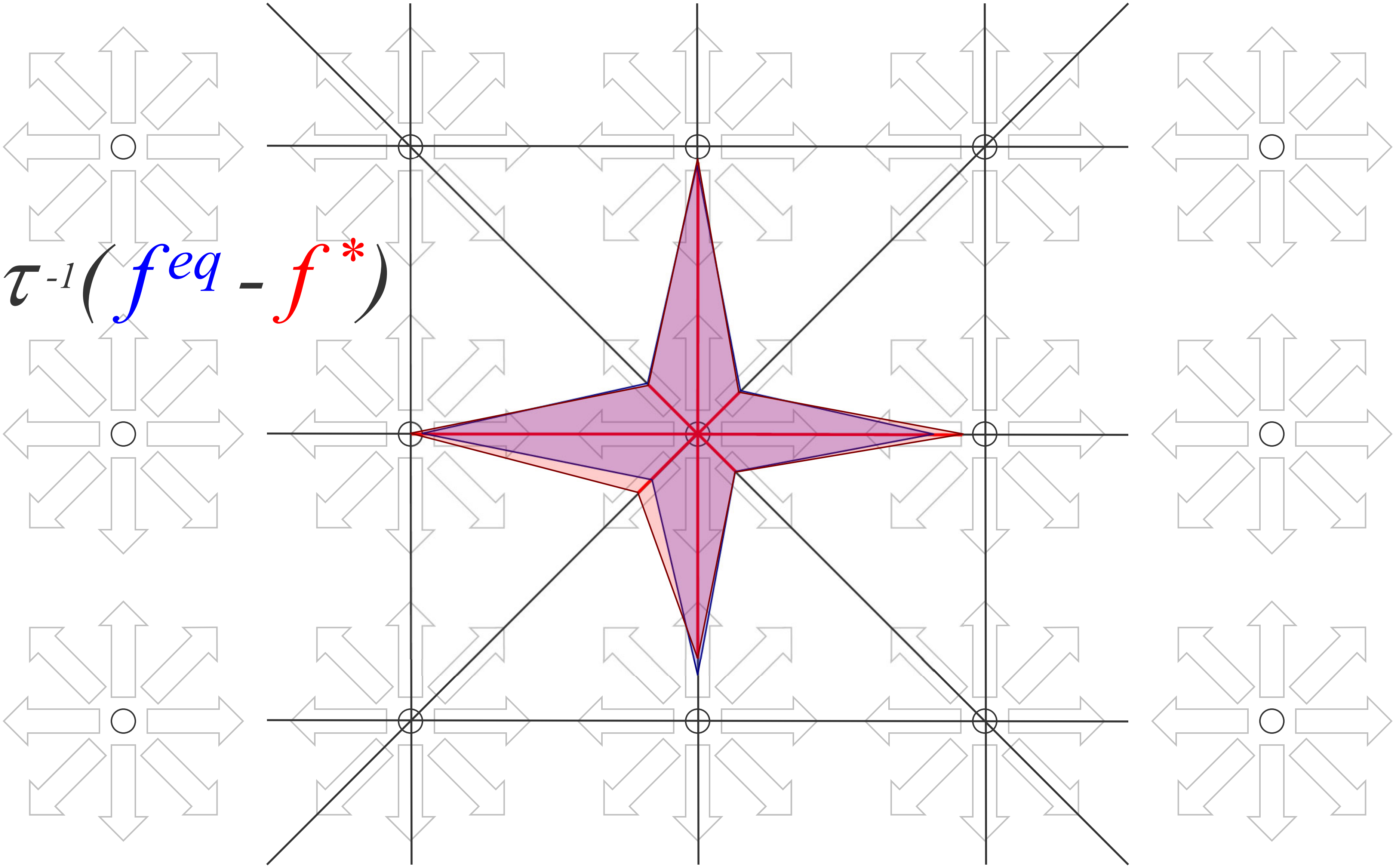
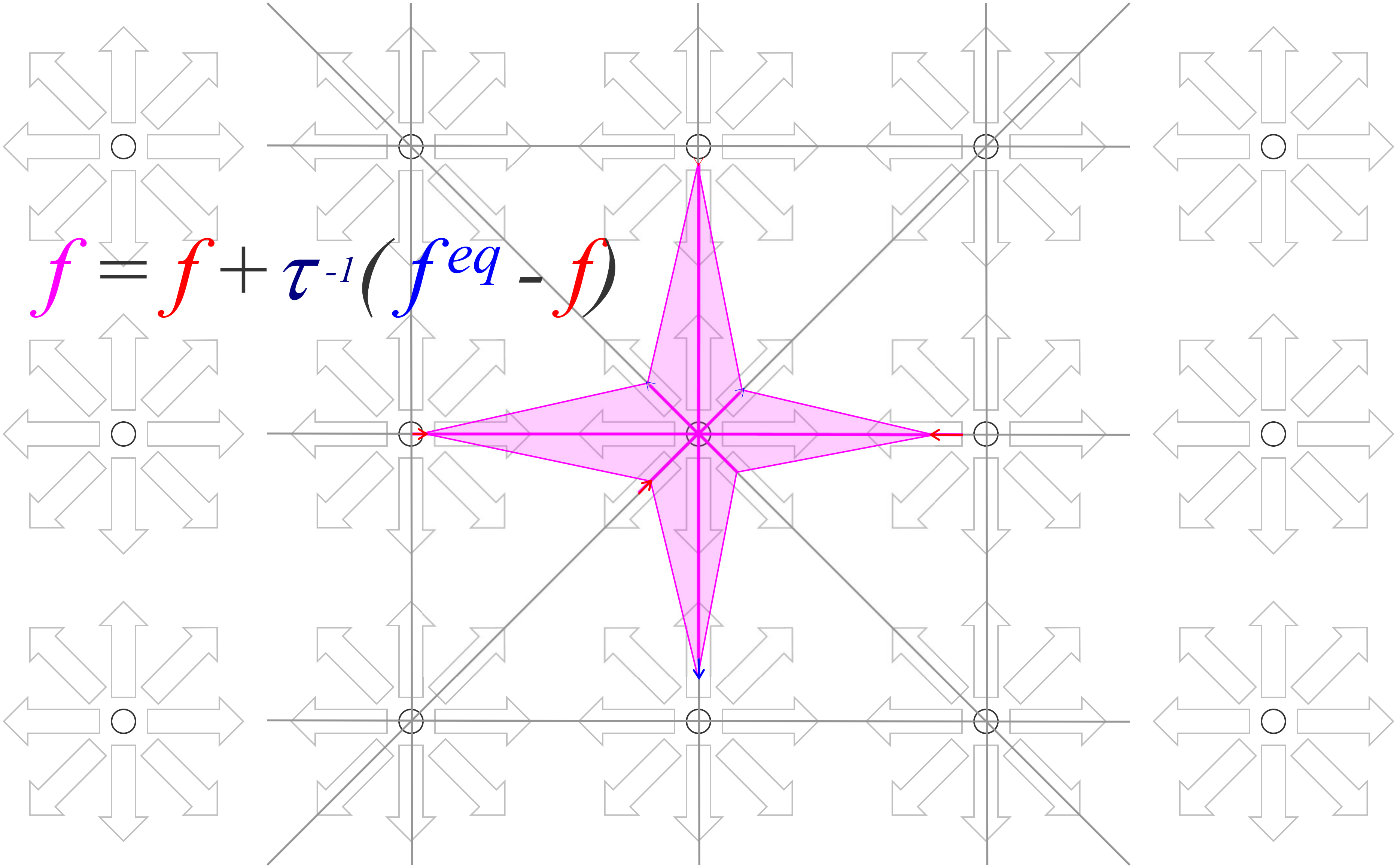
collision step



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

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

collision step



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

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

collision step

LBE 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 (small Ma=u/c_s) limit you get the

speed of sound

$$c_s = \frac{1}{\sqrt{3}}\frac{\Delta x}{\Delta t}$$

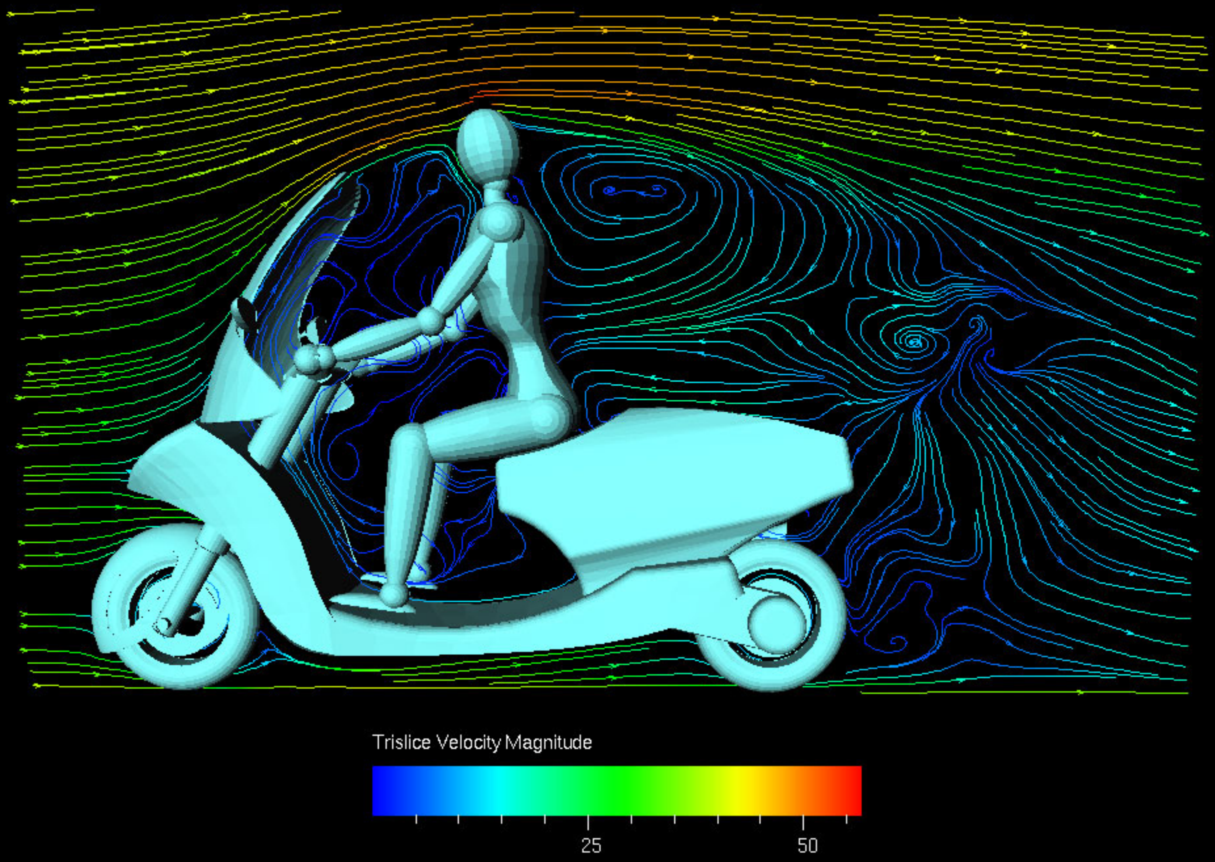
Navier Stokes equation

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

with

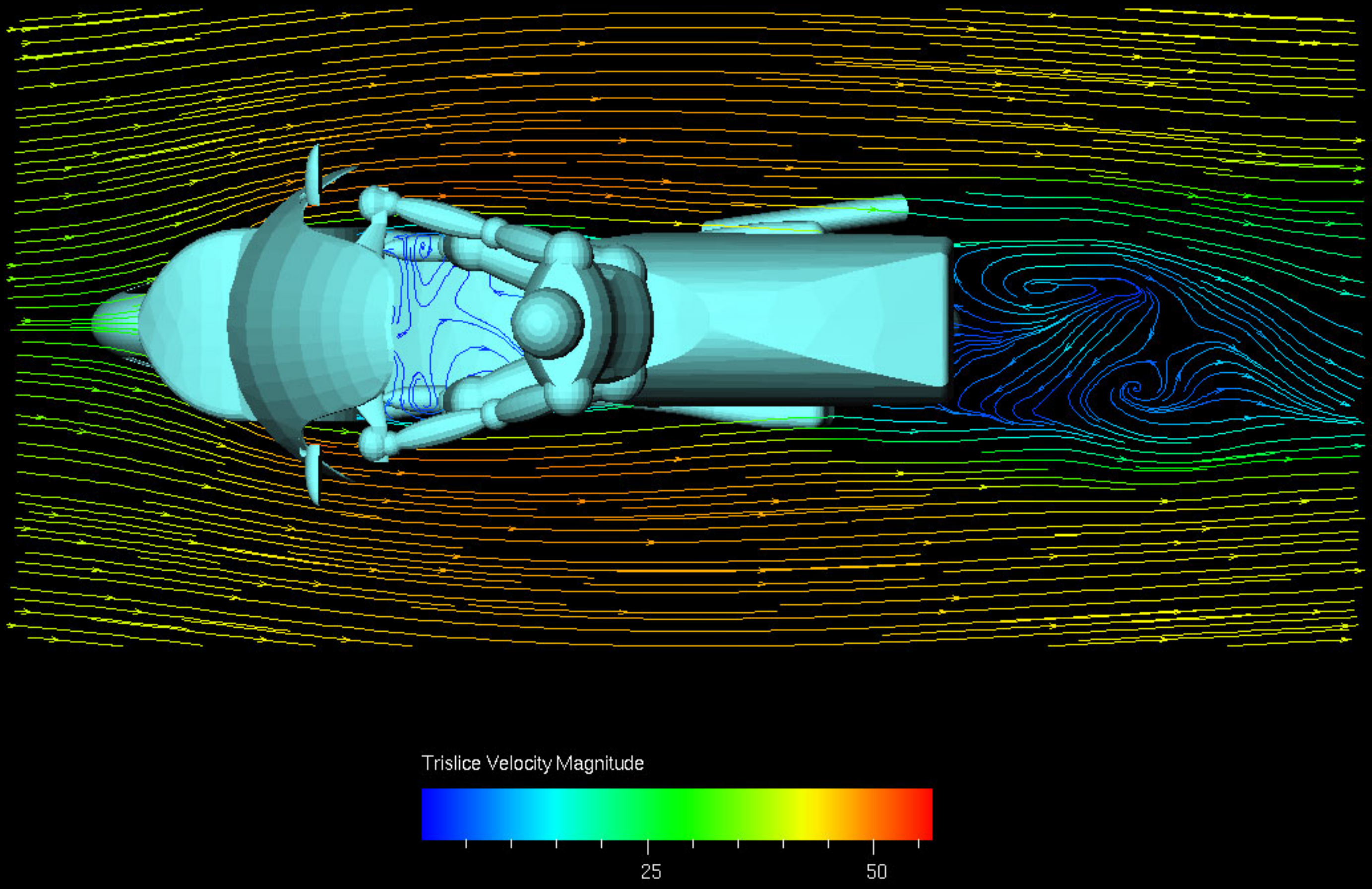
$$\nu = (\tau - \frac{1}{2})\frac{\Delta t}{3}$$

Examples (1)



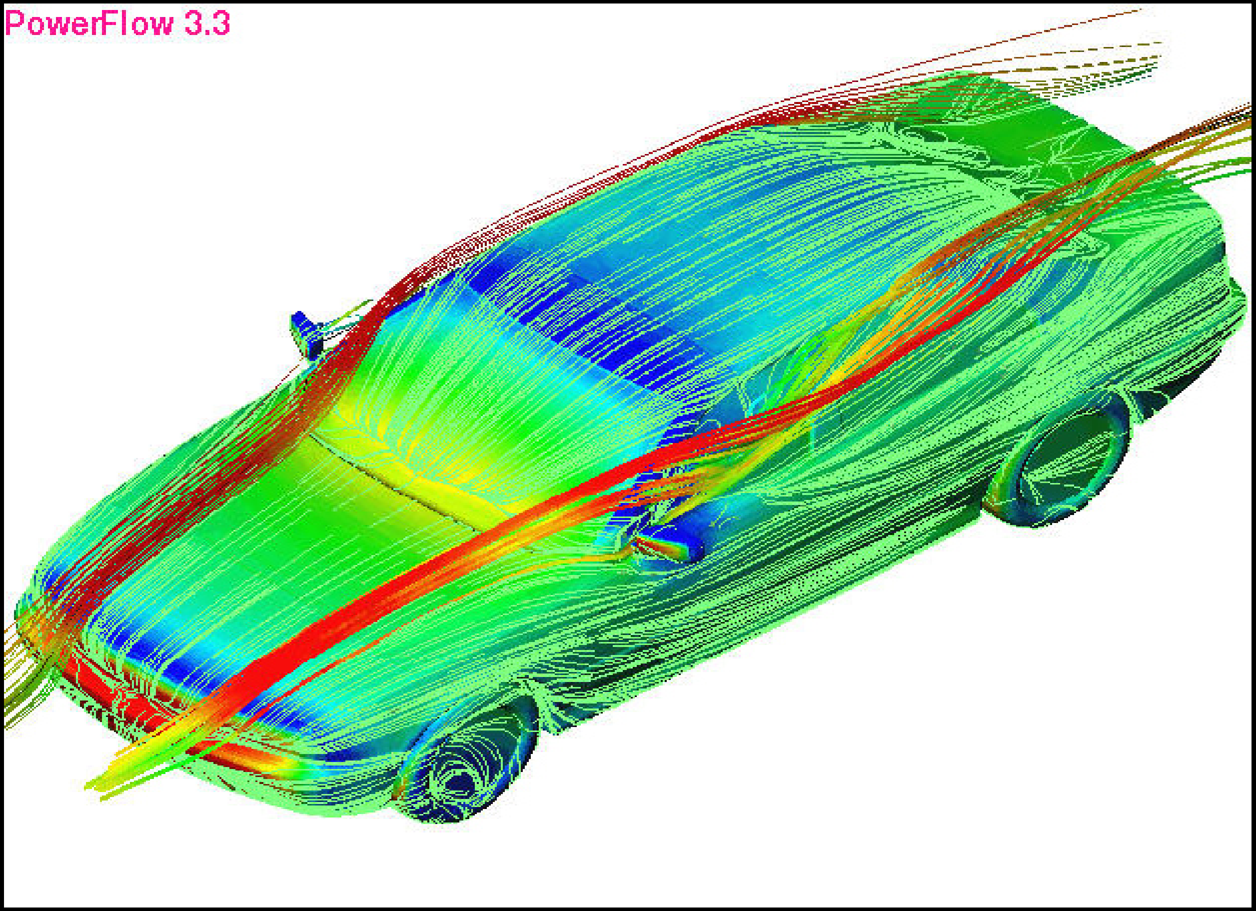
Bella, Ubertini,Succi 2001

Examples (1)



Bella, Ubertini,Succi 2001

Examples (2)



H Chen, S Kandasamy, R Shock, S. Orszag, S. Succi, V. Yakhot, Science (2003)

External forces

The acceleration of external forces (such as gravity) is incorporated in a velocity term

$$\mathbf{F} = m\mathbf{a} = m\frac{d\mathbf{u}}{dt}$$

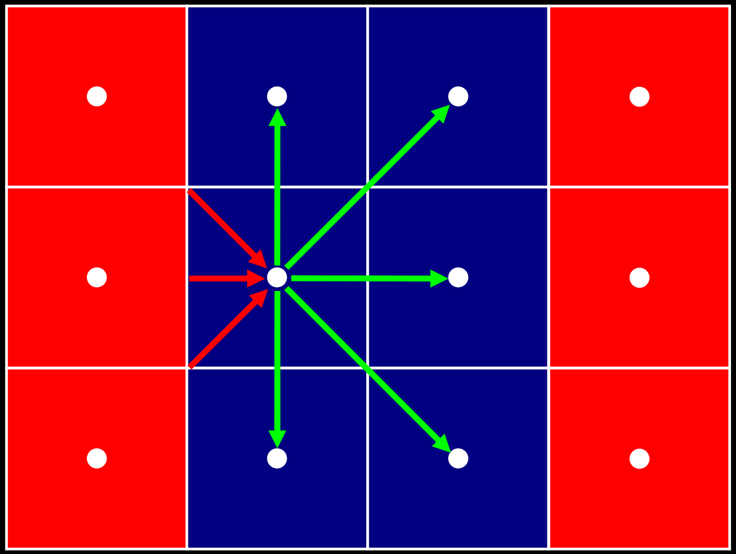
$$\Delta\mathbf{u} = \frac{\Delta t\mathbf{F}}{\rho}$$

$$\mathbf{u}^* = \mathbf{u} + \Delta\mathbf{u} = \sum_i f_i(\mathbf{r},t)\mathbf{c}_i + \frac{\Delta t\mathbf{F}}{\rho}$$

and then the new **u*** is used to construct the equilibrium distribution

Solid-fluid boundaries

Bounce-back rules



Summary

Lattice-Boltzmann method is

- a computational approach based upon particle movement and collisions.
- easy to implement and parallelize thanks to the local dynamics
- simple, flexible and able to incorporate complex boundary conditions

It may also be used to simulate the fluid with immersed moving objects (suspensions, polymers etc.)

References

- Sauro Succi „The Lattice Boltzmann equation", Oxford University Press, 2001
- S. Chen and G. Doolen, „Lattice Boltzmann method for fluid flows", Ann. Rev. Fluid. Mech, 30:329, 1998