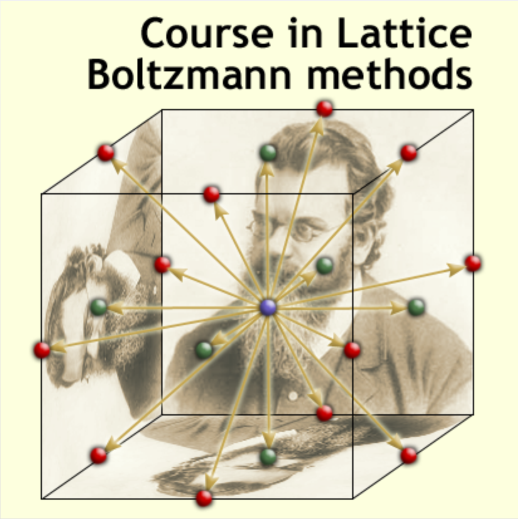
Lattice Boltzmann for multi-dimensional fluids



Sauro Succi

LB For fluids: d>1

The general idea of LB is to write down a set of hyperbolic equations for a discrete set of movers ("**fluons**") obeying a **Propagation-Relaxation** dynamics around prescribed local equilibria. Suitable choices of the equilibria lead to a broad variety of linear and non-linear PDE's.
A major advantage of the Prop-Relax dynamics is that it always proceeds along straight lines, no matter how complex the physics of the emergent PDE's.
The method is especially useful for the Navier-Stokes fluid equations for quasi-incompressible flows in d=1,2,3, which we now proceed to illustrate with special focus on the **symmetry requirements in d>1**.
Since LB was firts devised as an alternative fluid solver we start with a brief reminder of fluid dynamics

Navier-Stokes equations

- **Basic equations are known for nearly 2 centuries**

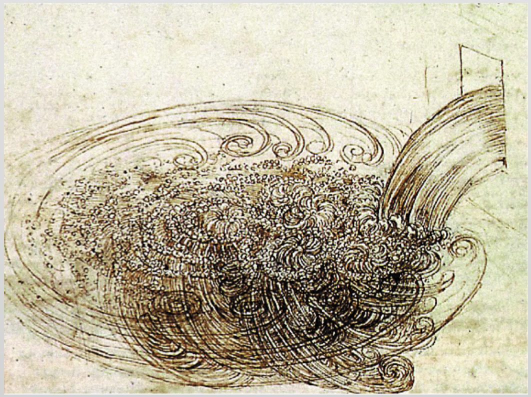
(L. Da Vinci)

$$\partial_t \vec{u} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \upsilon \Delta \vec{u}$$

$$\nabla \cdot \vec{u} = 0$$

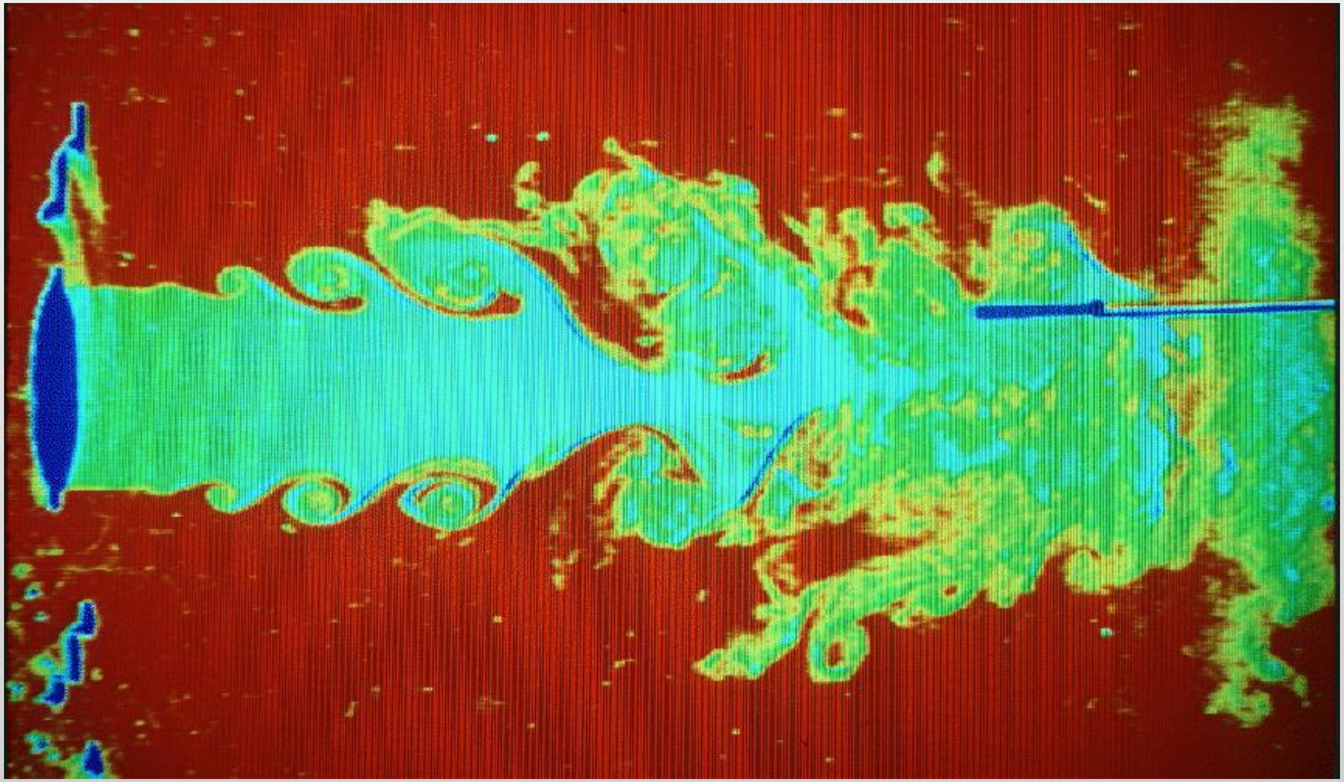
Reynolds number

$$\mathrm{Re} = \frac{UL}{\upsilon}$$



Turbulence!

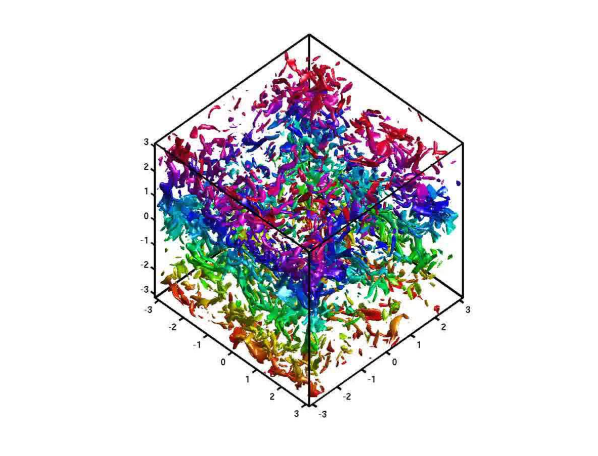
$$\mathrm{Re} \to \infty$$



The scales of turbulence

- **Kolmogorov length**

$$l_k = L / \mathrm{Re}^{3/4}$$



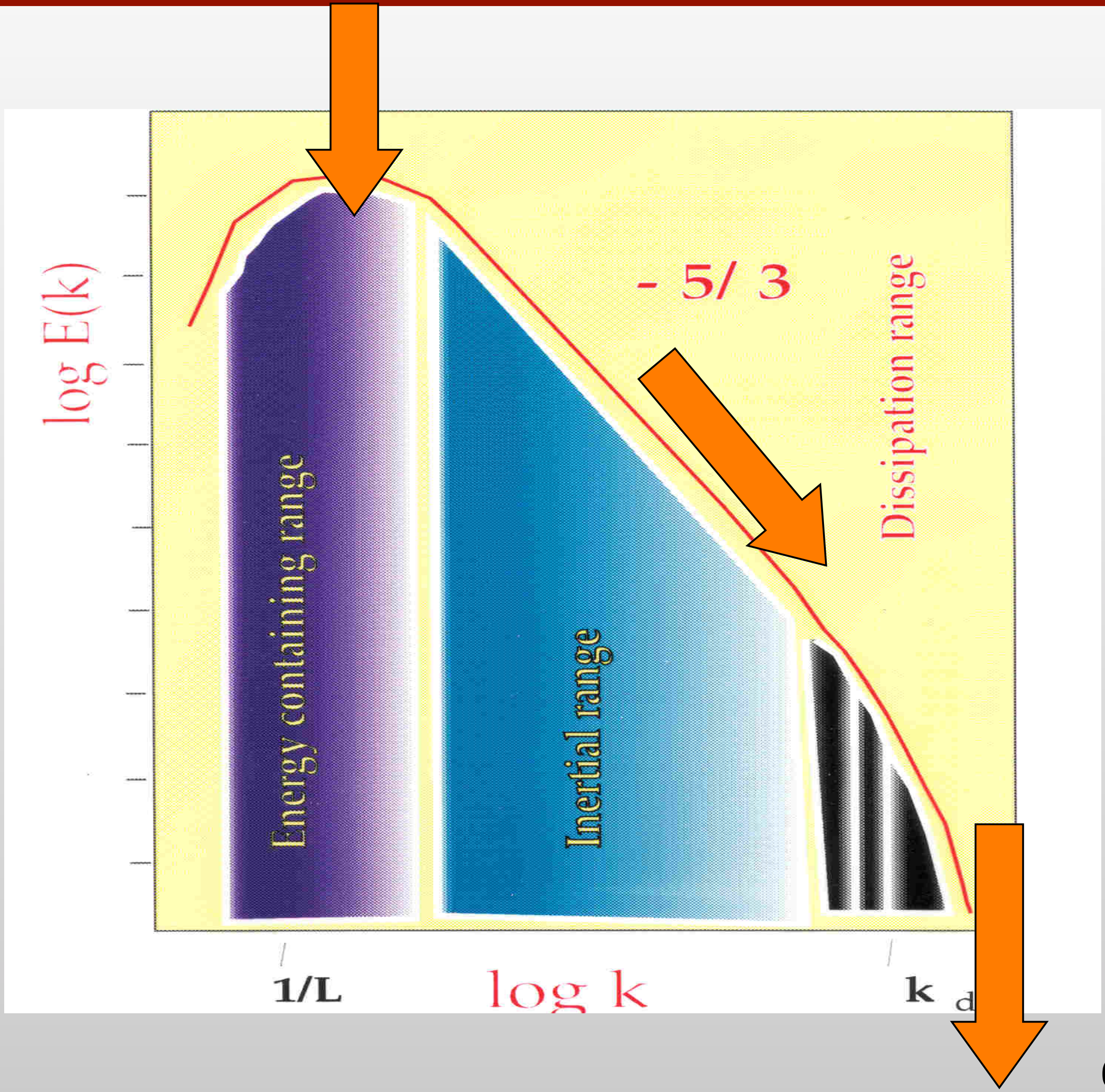
$$DOF = (L/l)^3 = \mathrm{Re}^{9/4}$$

Faucet, Re=10^4, DOF=10^9
Car/Airpl, Re=10^6-8, DOF=10^14-18
Geo/Astro, Re=10^10, DOF=10^22

Energy spectrum: broad and gapless!

Energy Cascade

Energy injected
at large scales
is transferred
to small scales
by nonlinearity
with virtually zero
dissipation.
Until structures
are small enough
for dissipation to
prevail: **Re=1.**
Then, coherence
is lost to "heat".
End of the
Energy Cascade



Navier-Stokes in d-dimensions

Coordinate representation:

$$\partial_t \rho + \partial_a(\rho u_a) = 0$$

$$\partial_t(\rho u_a) + \partial_b P_{ab} = F_a \qquad a, b = x, y, z$$

$$P_{ab} = \rho u_a u_b + p\delta_{ab} - \sigma_{ab}$$

Advection **Pressure** **Dissipation**

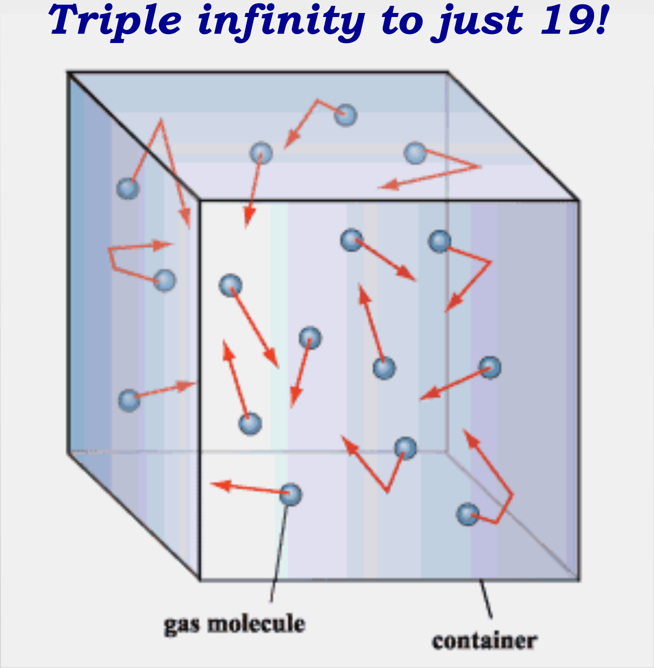
# of Macrofields= Constraints:

$$N_C = 1 + d + d(d+1)/2 = \{3, 6, 10\}$$

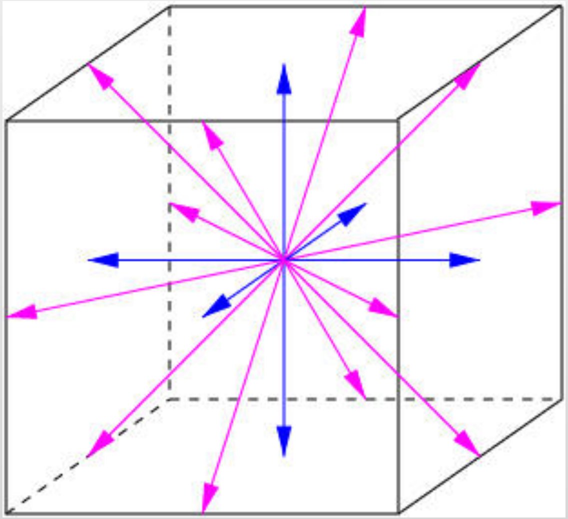
Lattice Boltzmann: Platonic hydrodynamics

$$\boxed{f(\vec{r},\vec{p};t) = \sum_{i=0}^{b} f_i(\vec{r},t)\delta(\vec{p}-\vec{c}_i)} \qquad i = 0, b$$

Triple infinity to just 19!



Magic speeds!



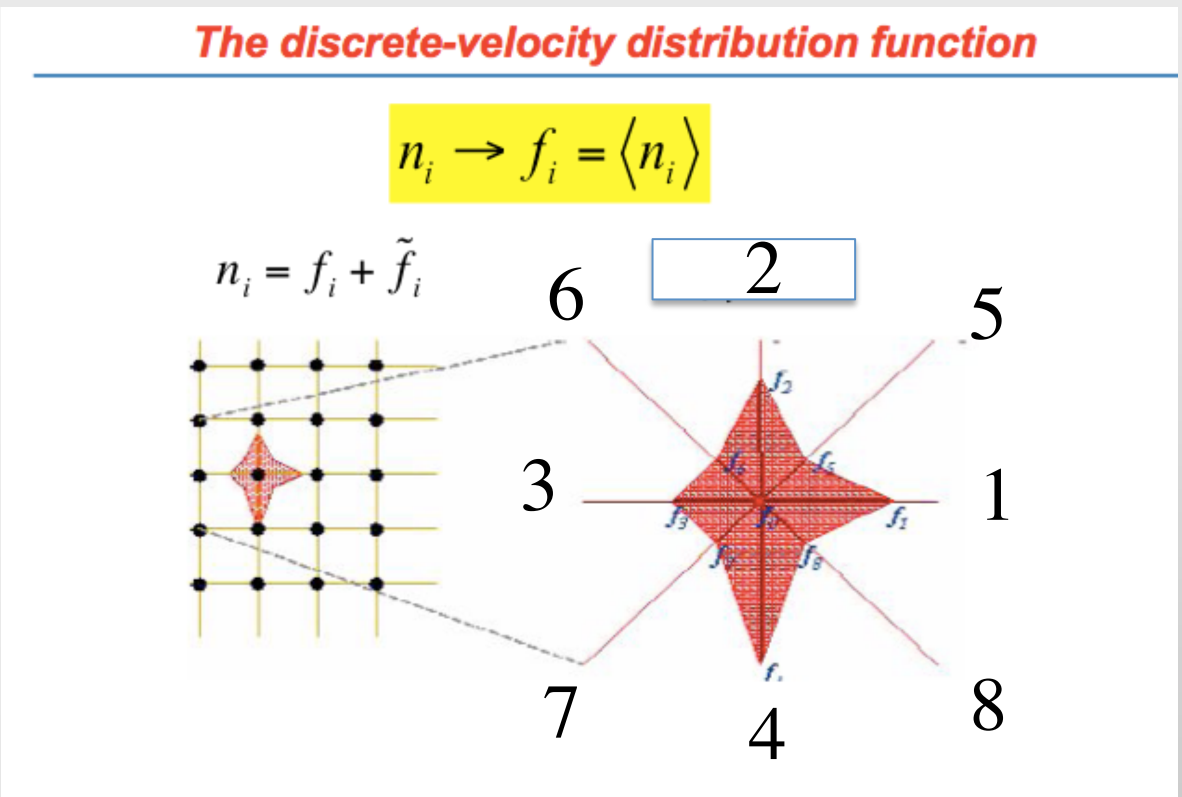
Exact sampling of frequent events

$$\rho(\vec{r};t) = \int f(\vec{r},\vec{p};t)\,d\vec{p} = \sum_{i=0}^{b} f(\vec{r},\vec{c}_i;t)$$

Lattice String Theory (?)

At each point in space (**x,y**) we have **8** arrows of magnitude **f_i** along direction **theta_i**. By joining the heads of the 8 arrows we obtain a closed contour (**string**). As time unfolds the contour changes it shape (string dynamics).

$$f(\vartheta;t) = \sum_{i=0}^{8} f_i(t)\delta(\vartheta - \vartheta_i)$$



$$\vartheta_{\{1,2,3,4\}} = \{0,1,2,3\}\pi/2$$

$$p_{\{1,2,3,4\}} = 1$$

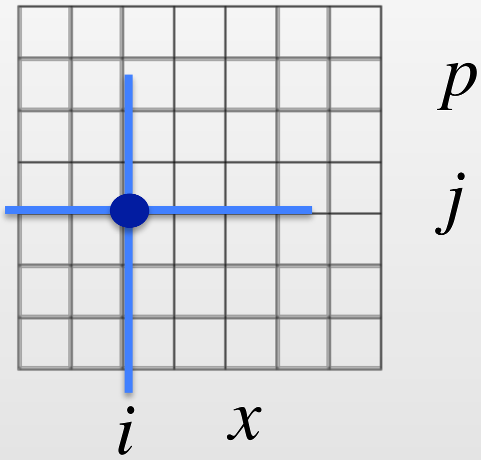
$$\vartheta_{\{5,6,7,8\}} = \{1,3,5,7\}\pi/4$$

$$p_{\{5,6,7,8\}} = \sqrt{2}$$

Sampling versus discretization

Discretization

$$f(\vec{r},\vec{p};t) \Rightarrow f_{ij}(t)$$



If the same resolution, N, is adopted in real and momentum space:

$$i = 1, N^d \quad j = 1, N^d$$

In **d+d** dimensions: $DoF = N^{2d}$

The best one can afford today is about 64^6=2^36=64 billion nodes in phase-space

But does momentum space demand the same resolution as real space? ***NO!***

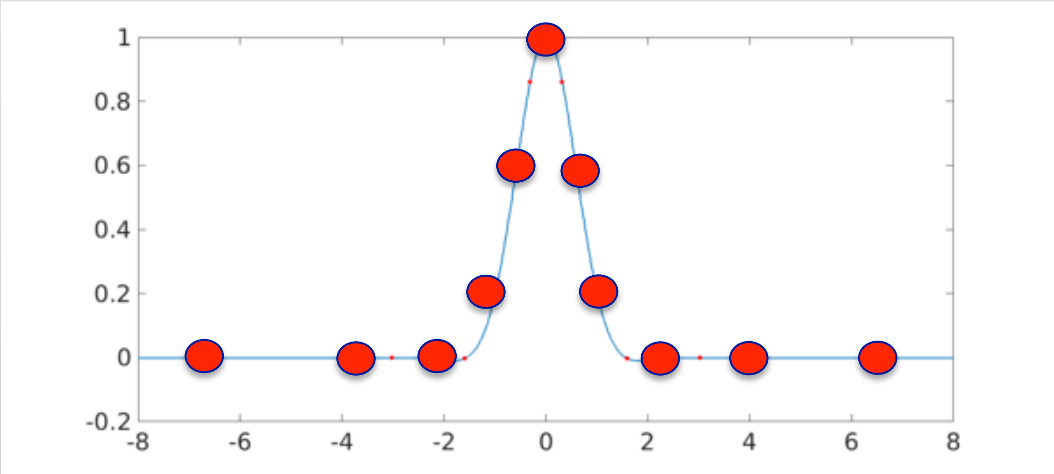
WHY? Collision Invariants

Sampling versus discretization

Gauss –Hermite quadrature

$$\int_{-\infty}^{+\infty} e^{-y^2/2} p(y)dy = \sum_{i=0}^{b} w_i p(y_i)$$

With the proper set of A FEW nodes x_i and weights w_i
The above relation is EXACT, NO DISCRETIZATION error!

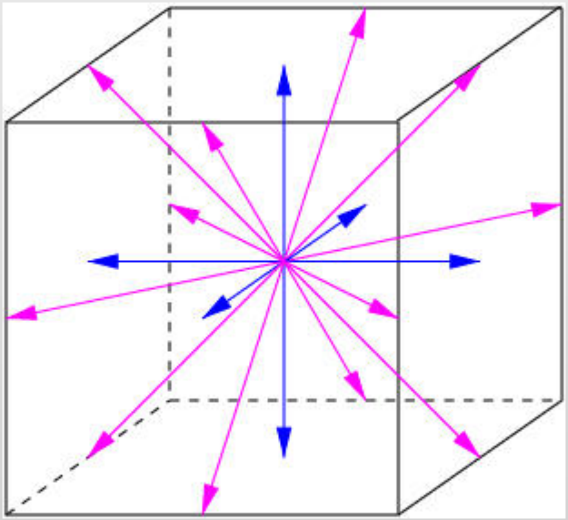


LB in d-dimensions

$$f_i(\vec{r} + \vec{c}_i \Delta t; t + \Delta t) - f_i(\vec{r}; t) = -\Omega_{ij} \Delta t (f_j - f_j^{eq})$$

$$i = 0, \boxed{2d < b < 3^d}$$

How to find:
c_i, Omega_ij , f_i^eq
In d-dimensions?



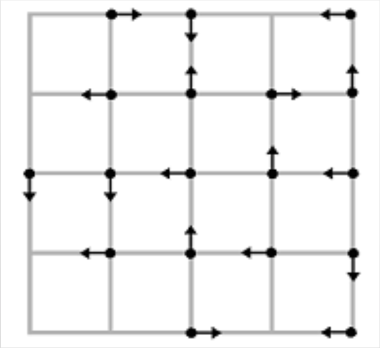
Lattice BGK (single-time relaxation)

$$\Omega_{ij} = \Omega \delta_{ij}$$
$$\omega = \Omega \Delta t = \Delta t / \tau$$

Navier-Stokes in d=2 dimensions

$$Hydro = \{\rho; u_x, u_y; P_{xx}, P_{xy}, P_{yy}\}$$

D2Q4=HPP (1976)



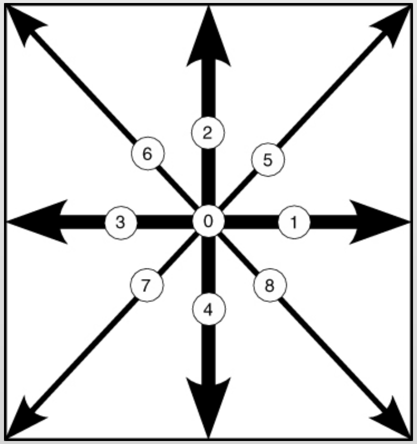
$$\vec{c}_1 = (1,0) \qquad \vec{c}_2 = (0,1)$$

$$\vec{c}_3 = (-1,0) \qquad \vec{c}_4 = (0,-1)$$

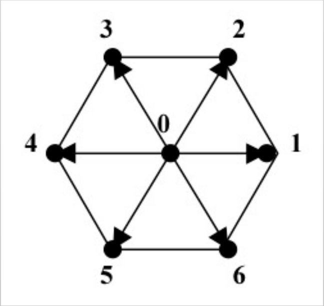
$$c_{ix}c_{iy} = 0 \Rightarrow u_a u_b = 0$$ NO!

Natural: 4 speeds versus 6 macrofields: no way!

But 9 is better (D2Q9)



D2Q6=FHP (1986)



$$c_{ix}c_{iy} \neq 0 \Rightarrow u_a u_b \neq 0$$ YES!

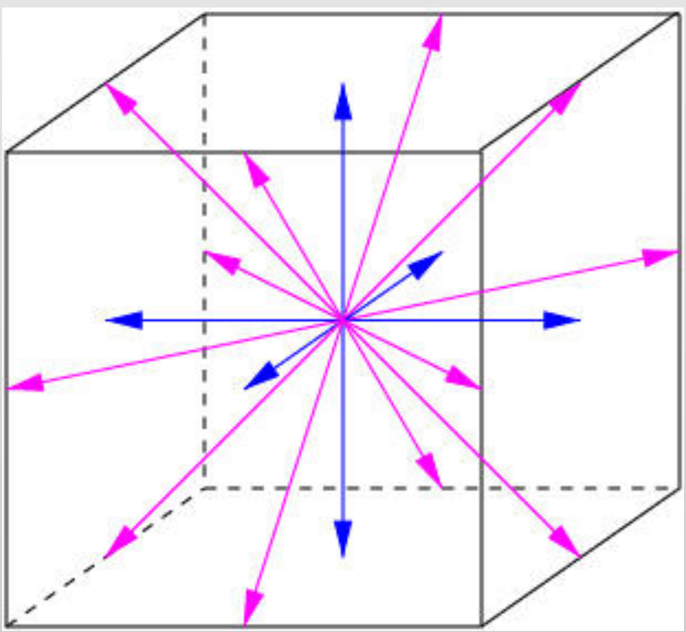
Natural: 6 speeds versus 6 macrofields: ok!

Navier-Stokes in d=3 dimensions

$$Hydro = \{\rho; u_x, u_y, u_z; P_{xx}, P_{xy}, P_{xz}, P_{yy}, P_{yz}, P_{zz}\}$$

$$f_i = \{Vx = \pm c; Vy = \pm c, Vz = \pm c\}$$

6 speeds vs 10 fields: NO WAY!



D3Q19: YES!
10 hydrofields + 9 “ghosts”

D3Q27: yes, of course

Moment matching

Moment matching proceeds exactly as in d=1, with algebraic aggravation due to the **tensorial structure** of fluid dynamics: **Rotational Invariance** must be secured. A crucial step is to recognize that the expansion is the lattice analogue of the **Hermite expansion** in continuum kinetic theory. This simplifies enormously moment-matching procedure and puts it on a systematic basis.

Let us take a close look at the procedure.

Moment matching: Mass

Start from LB in differential BGK form:

$$\partial_t f_i + c_{ia}\partial_a f_i = -\Omega(f_i - f_i^{eq})$$

Mass, sum over all discrete speeds:

$$\partial_t(\sum_i f_i) + \partial_a(\sum_i c_{ia} f_i) = -\Omega \sum_i (f_i - f_i^{eq})$$

$$\partial_t \rho + \partial_a J_a = -\omega(\rho - \rho^{eq})$$

$$\sum_{i=0}^{b} f_i = \rho$$

$$\sum_{i=0}^{b} f_i\, c_{ia} = J_a \equiv \rho u_a$$

By imposing: $\boxed{\rho^{eq} = \rho}$

$$\boxed{\partial_t \rho + \partial_a(\rho u_a) = 0}$$

Moment matching: Momentum

$$\partial_t f_i + c_{ib}\partial_b f_i = -\Omega(f_i - f_i^{eq})$$

Momentum: multiply by c_ia and sum over all discrete directions:

$$\partial_t(\sum_i f_i c_{ia}) + \partial_b(\sum_i c_{ia}c_{ib}f_i) = -\Omega\sum_i c_{ia}(f_i - f_i^{eq})$$

$$\partial_t(\rho u_a) + \partial_b P_{ab} = -\Omega(J_a - J_a^{eq})$$

$$\sum_{i=0}^{b} f_i\, c_{ia} = J_a \equiv \rho u_a$$

By imposing: $\boxed{J_a^{eq} = J_a}$

$$\sum_{i=0}^{b} f_i\, c_{ia}c_{ib} \equiv P_{ab}$$

$$\partial_t(\rho u_a) + \partial_b P_{ab} = 0$$

Is it Navier-Stokes? **NOT YET! Constraints must be imposed on P_ab**

Moment matching: momentum

The Navier-Stokes pressure tensor without
Dissipation (inviscid Euler regime)

$$P_{ab}^{Euler} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} \equiv \rho u_a u_b + p\delta_{ab}$$

Advection + Pressure

Dissipation is the macroscopic Manifestation of non-equilibrium!

Moment matching: Momflux

$$\partial_t f_i + c_{ic}\partial_c f_i = -\Omega(f_i - f_i^{eq})$$

Momentum flux, multiply by c_{ia}c_{ib} and sum over i:

$$\partial_t(\sum_i f_i c_{ia} c_{ib}) + \partial_c(\sum_i c_{ia} c_{ib} c_{ic} f_i) = -\omega \sum_i c_{ia} c_{ib}(f_i - f_i^{eq})$$

$$\partial_t P_{ab} + \partial_c Q_{abc} = -\Omega(P_{ab} - P_{ab}^{eq})$$

$$\sum_{i=0}^{b} f_i\, c_{ia} c_{ib} \equiv P_{ab}$$

Now $P_{ab} \neq P_{ab}^{eq}$ because momflux is **not a** micro-invariant!

$$\sum_{i=0}^{b} f_i\, c_{ia} c_{ib} c_{ic} \equiv Q_{abc}$$

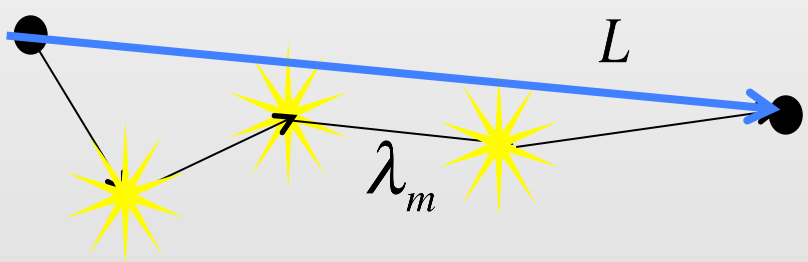
$$\partial_t P_{ab} + \partial_c Q_{abc} = -\Omega(P_{ab} - P_{ab}^{eq})$$

How do we close this equation?

Boltzmann to Navier-Stokes

1. Scale separation:

The molecular mean free path must be much smaller than any hydrodynamic length-scale (small **Knudsen** number)



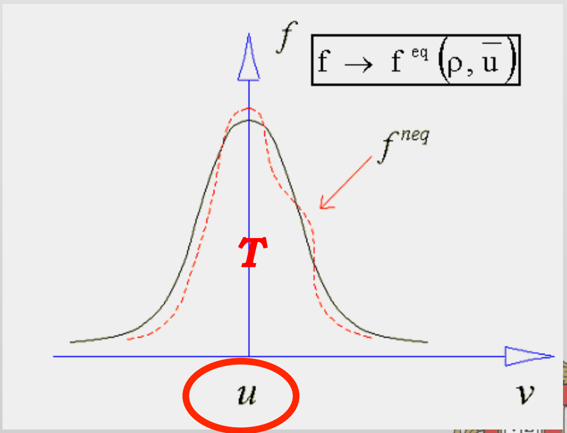
$$Kn = \frac{\lambda_m}{L} << 1$$

2. Weak departure from local equilibrium:

The Boltzmann probability distribution function must be close to a local Maxwell-Boltzmann

$$f = f^{eq} + f^{neq}$$

$$Kn \approx \frac{|f^{neq}|}{f^{eq}} << 1$$



Momflux: enslaving

Momentum flux equation:

$$\partial_t P_{ab} + \partial_c Q_{abc} = -\Omega(P_{ab} - P_{ab}^{eq})$$

Enslaving: eliminate time derivative on a timescale tau=1/omega:

$$P_{ab} \approx P_{ab}^{eq} - \tau \partial_c Q_{abc}$$

Close to local equil: $Q_{abc} \approx Q_{abc}^{eq}$

$$P_{ab} \approx P_{ab}^{eq} - \tau \partial_c Q_{abc}^{eq}$$

Dissipation

Inertia+Pressure

Momflux: enslaving

Injecting $P_{ab} \approx P_{ab}^{eq} - \tau \partial_c Q_{abc}^{eq}$ into the momentum equation, we obtain:

$$\partial_t J_a + \partial_b (P_{ab}^{eq} - \tau \partial_c Q_{abc}^{eq}) = 0$$

This must now match exactly the Navier-Stokes equations:

$$\partial_t (\rho u_a) + \partial_b (\rho u_a u_b + p\delta_{ab}) = \partial_b \sigma_{ab}$$

Which implies the following **tensorial** constraints:

$$P_{ab}^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} = \rho u_a u_b + p\delta_{ab}$$ **Inertia+Pressure**

$$\tau Q_{abc}^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} c_{ic} = \sigma_{ab}$$ **Dissipation**

List of hydrodynamic constraints

$$\rho^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} = \rho$$

Scalar: 1 constraint

$$J_a^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} = \rho u_a$$

Vector: d constraints

$$P_{ab}^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} = \rho u_a u_b + p\delta_{ab}$$

2-Tensor: d*(d+1)/2 constraints

$$Q_{abc}^{eq} \equiv \sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} c_{ic} = \sigma_{ab} / \tau$$

3-Tensor: d*(d+1)*(d+2)/6 constraints

Q: Can we match the full list? How many discrete velocities?

Lattice equilibria: constraints

$$\sum_{i=0}^{b} f_i^{eq} = \rho$$

Continuity equation

$$\sum_{i=0}^{b} f_i^{eq} c_{ia} = \rho u_a$$

Momentum Equation

$$\sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} = \rho u_a u_b + p\delta_{ab}$$

Pressure+Advection

Newtonian (linear) Dissipation

$$\sum_{i=0}^{b} f_i^{eq} c_{ia} c_{ib} c_{ic} = \rho c_s^2 (u_a \delta_{bc} + u_b \delta_{ac} u_b + u_c \delta_{ab})$$

Lattice Equilibria

Expand the local Maxwell-Boltzmann to second order in Mach number:

$$f_i^{eq} = w_i \rho (1 + u_i + \frac{1}{2} q_i + \ldots)$$

where:

$$u_i = \frac{c_{ia} u_a}{c_s^2} = \frac{\vec{u} \cdot \vec{c}_i}{c_s^2}$$

Projection of the flow field over the i-th discrete speed

$$q_i = \frac{(c_{ia} c_{ib} - c_s^2 \delta_{ab}) u_a u_b}{c_s^4} = u_i^2 - u^2 / c_s^2$$

$$Q_{iab} \equiv c_{ia} c_{ib} - c_s^2 \delta_{ab}$$

is a lattice projector along c_i direction

$$(\sum_i Q_{iab} \equiv \sum_i c_{ia} c_{ib} - c_s^2 \delta_{ab} = 0)$$

Question: **How do we find the optimal weights**?

Lattice Equilibria

By inserting

$$f_i^{eq} = w_i \rho (1 + u_i + \frac{1}{2} q_i)$$

in the list of hydrodynamic constraints, we obtain:

$$\sum_{i=0}^{b} w_i = 1$$

0th order isotropy

$$\sum_{i=0}^{b} w_i c_{ia} c_{ib} = c_s^2 \delta_{ab}$$

2nd order isotropy

$$\sum_{i=0}^{b} w_i c_{ia} c_{ib} c_{ic} c_{id} = c_s^4 (\delta_{ab} \delta_{cd} + Perm)$$

4th order isotropy

Lattice equilibria: Mass

Insert local equils: $f_i^{eq} = w_i \rho (1 + u_i + \frac{1}{2} q_i)$ into Mass Conservation:

$$\rho \{ \sum_{i=0}^{b} w_i + \frac{1}{c_s^2} (\sum_{i=0}^{b} w_i c_{ia}) u_a + \frac{1}{2c_s^4} (\sum_{i=0}^{b} w_i Q_{iab}) u_a u_b \} = \rho$$

$$\sum_{i=0}^{b} w_i = 1$$

Order 0: Normalization

$$\sum_{i=0}^{b} w_i c_{ia} = 0$$

Order 1: Guaranteed by mirror symmetry (**Parity Invariance**)

$$\sum_{i=0}^{b} w_i c_{ia} c_{ib} = c_s^2 \delta_{ab}$$

Order 2: defines the lattice sound speed

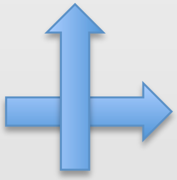
Higher Order Lattice equilibria

Expand the local Maxwell-Boltzmann to third order in Mach number:

$$f_i^{eq} = w_i \rho (1 + u_i + \frac{1}{2} q_i + \frac{1}{6} t_i + \ldots)$$

$$u_i = \frac{u_a c_{ia}}{c_s^2}$$

Dipole u_a

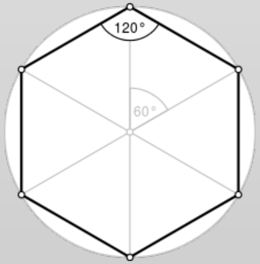


$$q_i = \frac{Q_{iab} u_a u_b}{c_s^4}$$

Quadrupole $u_a u_b$

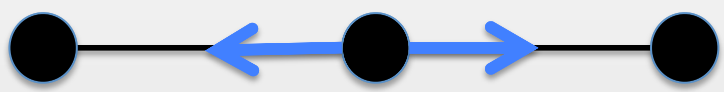
$$Q_{iab} \equiv c_{ia} c_{ib} - c_s^2 \delta_{ab}$$

Hexapole:



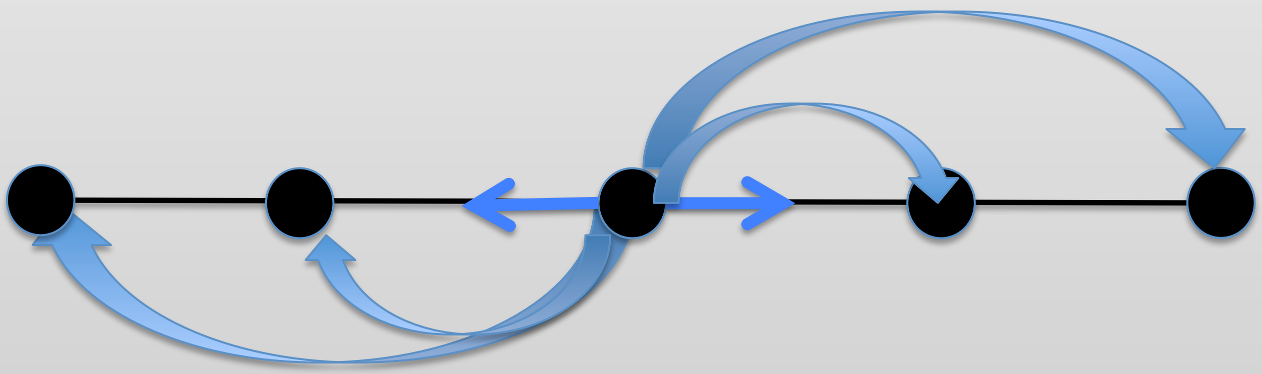
$$t_i = \frac{[c_{ia} c_{ib} c_{ic} - c_s^2 (c_{ia} \delta_{bc} + c_{ib} \delta_{ac} + c_{ic} \delta_{ab}) u_a u_b u_c}{c_s^6}$$

D1 lattice equilibria



D1Q3

$$c_{ix} = \{-1,0,1\} \quad w_i = \frac{1}{6}\{1,4,1\} \quad c_s^2 = 1/3$$



D1Q5

$$c_{ix} = \{-2,-1,0,+1,+2\}$$

Compute D2Q9 equilibria

Linear (Dipole)

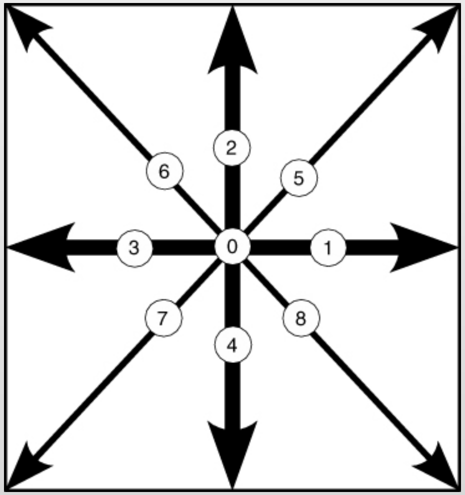
$$c_s^2 = 1/3$$

$$u_0 = 0$$

$$u_1 = +3u_x \qquad u_2 = +3u_y \qquad u_3 = -3u_x \qquad u_4 = -3u_y$$

$$u_5 = +3(u_x + u_y) \qquad u_6 = +3(-u_x + u_y)$$

$$u_7 = -3(u_x + u_y) \qquad u_8 = +3(u_x - u_y)$$



Quadratic (quadrupole)

$$Q_{ixx} = c_{ix}^2 - 1/3 \qquad Q_{ixy} = c_{ix}c_{iy} \qquad Q_{iyy} = c_{iy}^2 - 1/3$$

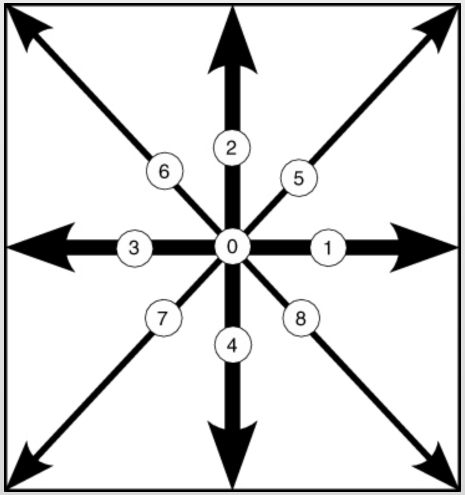
$$q_i = Q_{ixx}u_x^2 + 2Q_{ixy}u_x u_y + Q_{iyy}u_y^2$$

D2Q9 equilibria

$$w_i = \{\frac{4}{9}; \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}; \frac{1}{36}, \frac{1}{36}, \frac{1}{36}. \frac{1}{36}\} \qquad c_s^2 = 1/3$$

Quadratic polynomials (Check the algebra!):

$$f_0^{eq} = \frac{4\rho}{9}[1 - \frac{3}{2}(u_x^2 + u_y^2)]$$



$$f_1^{eq} = \frac{\rho}{9}(1 + 3u_x + 3u_x^2) \qquad f_3^{eq} = \frac{\rho}{9}(1 - 3u_x + 3u_x^2)$$

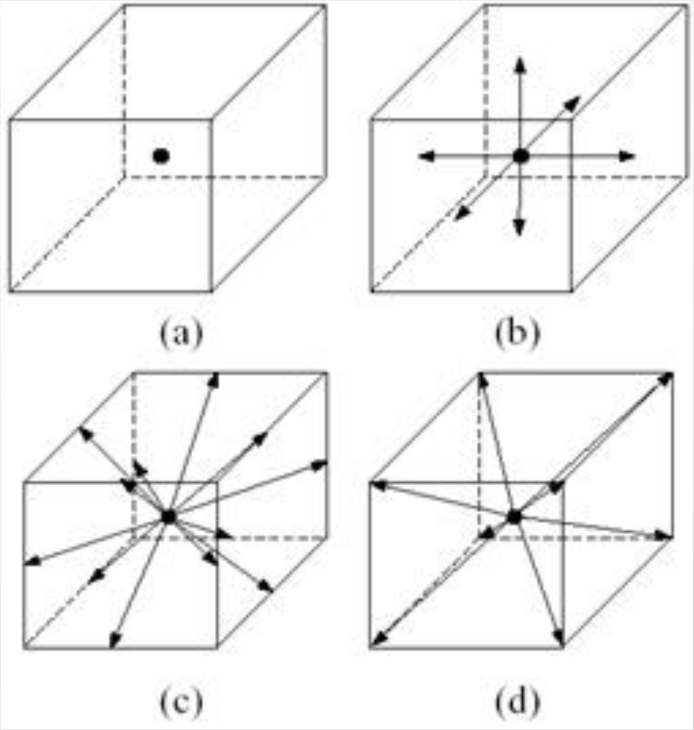
$$f_2^{eq} = \frac{\rho}{9}(1 + 3u_y + 3u_y^2) \qquad f_4^{eq} = \frac{\rho}{9}(1 - 3u_y + 3u_y^2)$$

$$f_5^{eq} = \frac{\rho}{36}(1 + 3u_x + 3u_y + 2u_x u_y) \qquad f_6^{eq} = \frac{\rho}{36}(1 - 3u_x + 3u_y - 2u_x u_y)$$

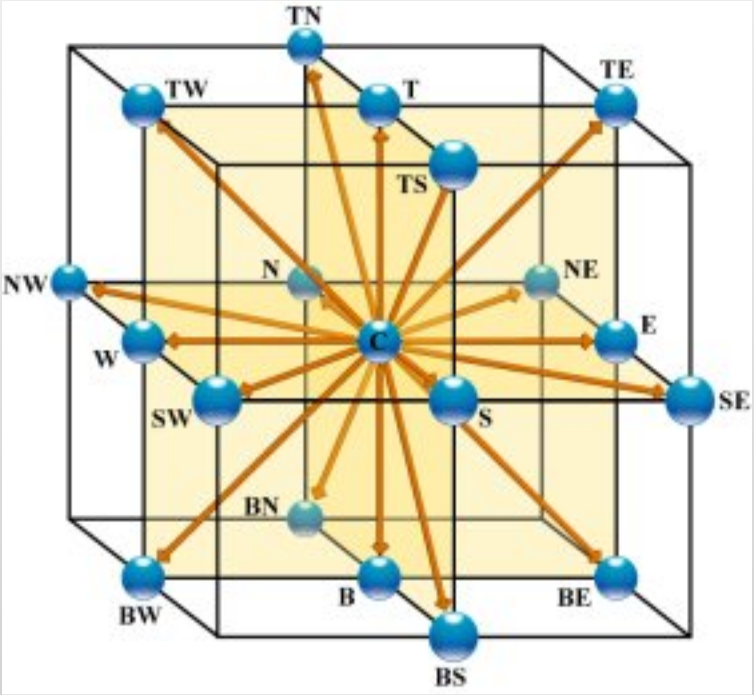
$$f_7^{eq} = \frac{\rho}{36}(1 - 3u_x - 3u_y + 2u_x u_y) \qquad f_8^{eq} = \frac{\rho}{36}(1 + 3u_x - 3u_y - 2u_x u_y)$$

Standard 3d LB lattices

D3Q27=(D1Q3)^3

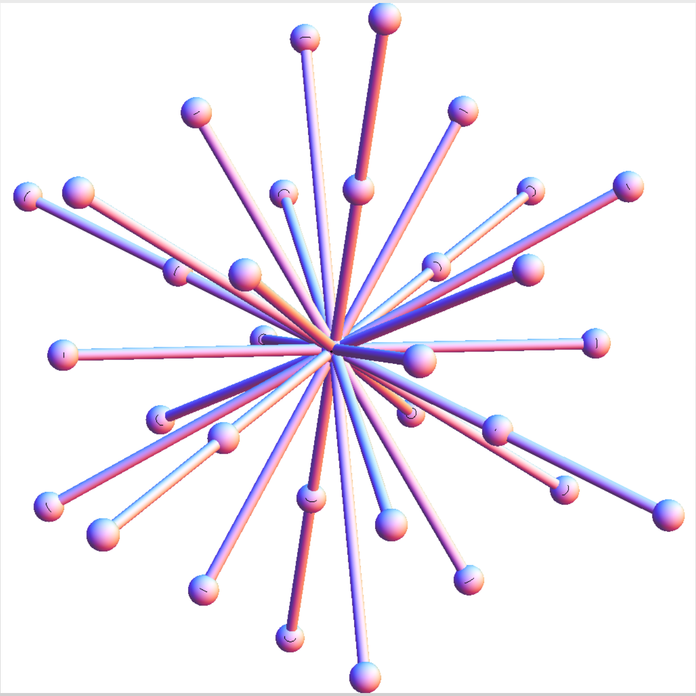


D3Q19= D3Q27-8 vertices

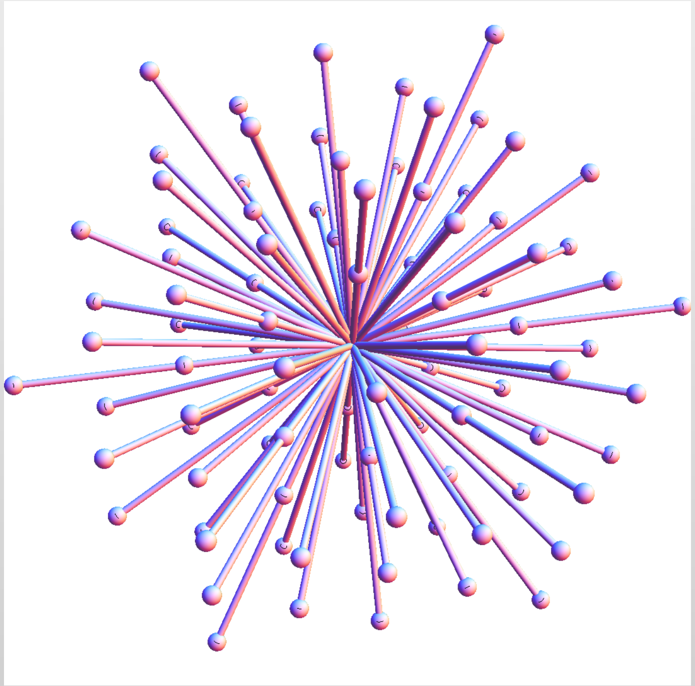


Higher order lattices

D3Q39: order 6 isotropy

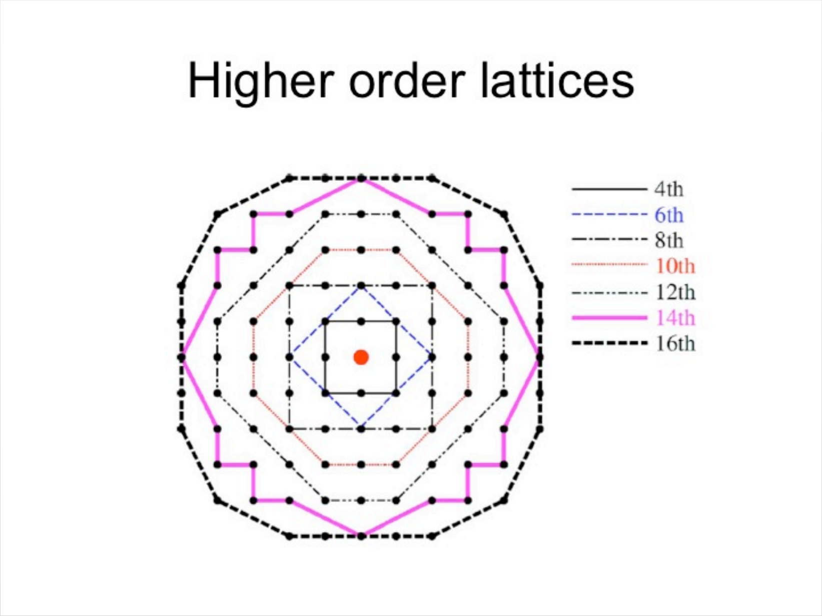


D3Q93: order 8 isotropy

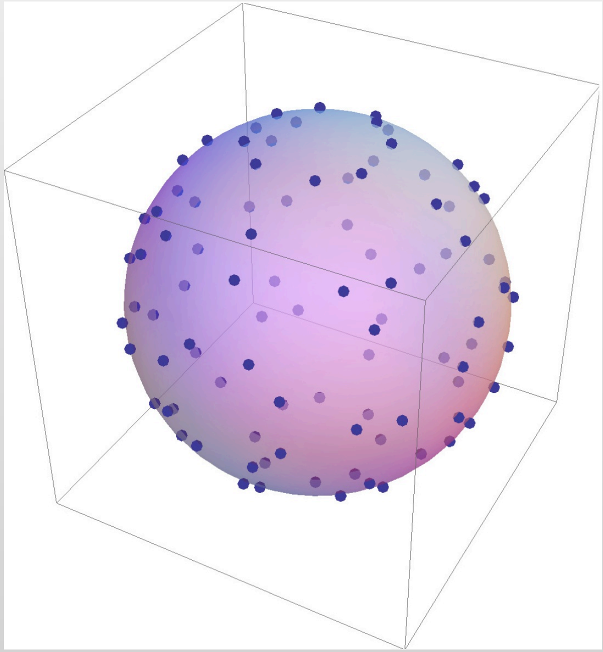


Very Higher Order Lattices

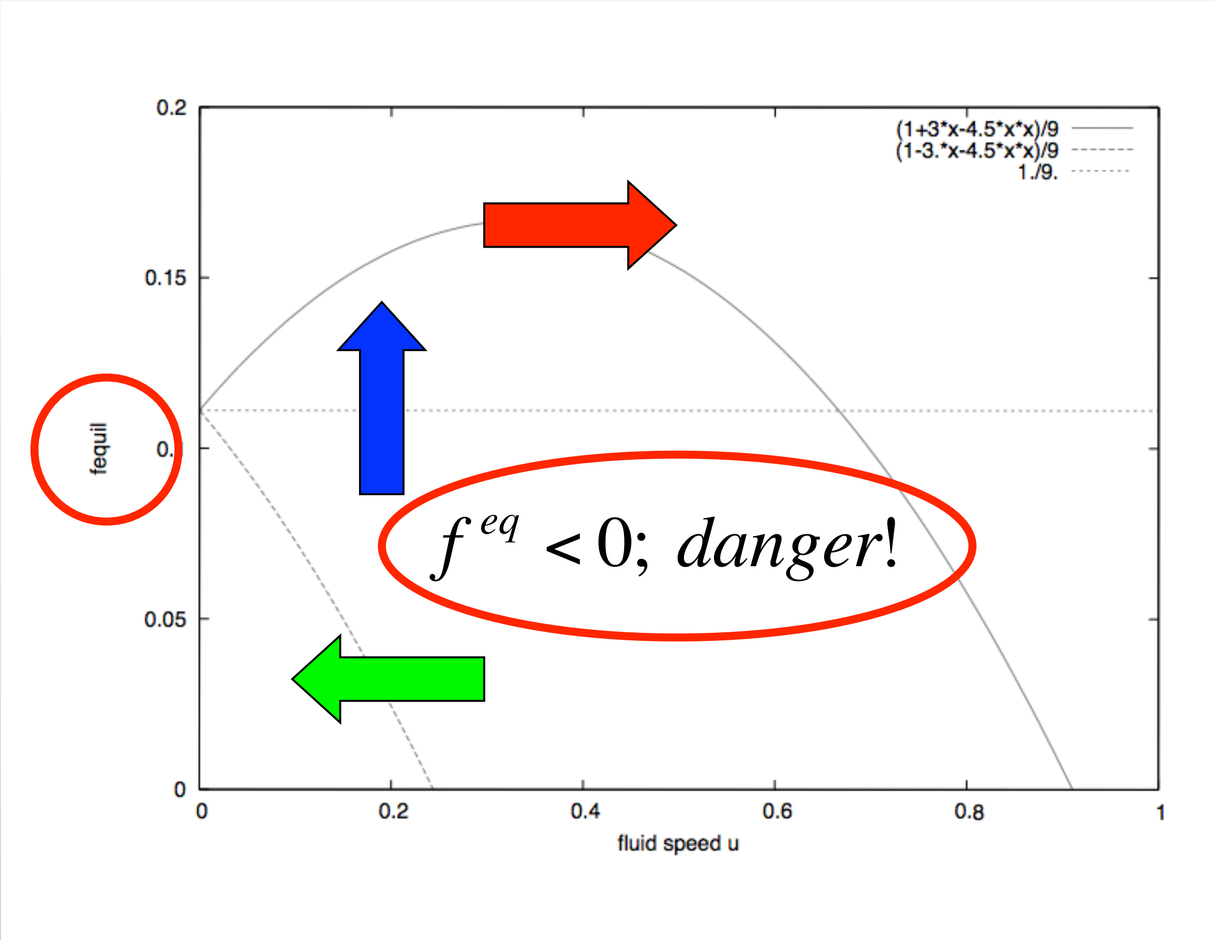
D=2, up to order 16!



D=3, relativistic



Realizability (positivity): Low Mach



The LB fluid must move slowly **u/cs <0.1**: **NEARLY INCOMPRESSIBLE!**

Summary

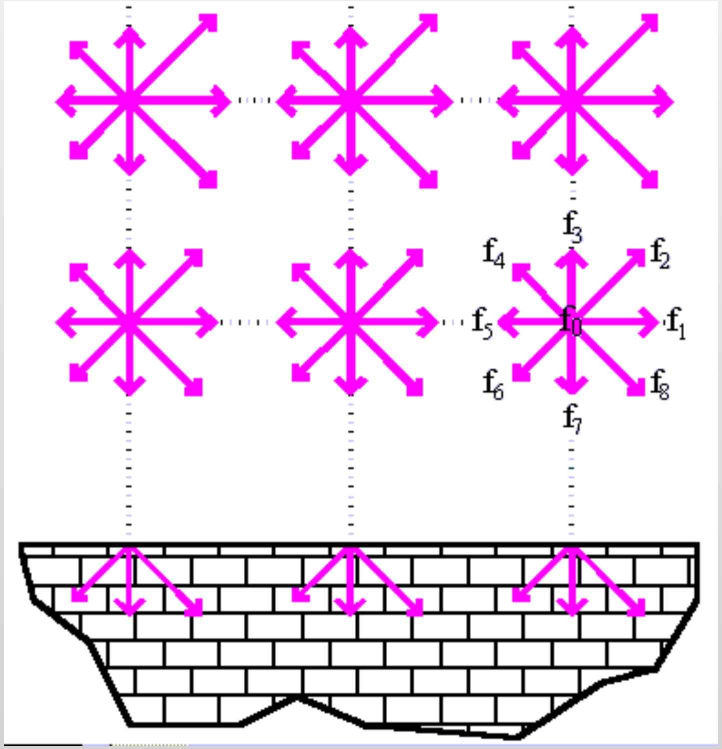
Summarizing: by choosing a suitable set of discrete velocities and associated weights, ensuring **fourth order isotropy**, the LBE reproduces the Navier-Stokes equations for a fluid with:

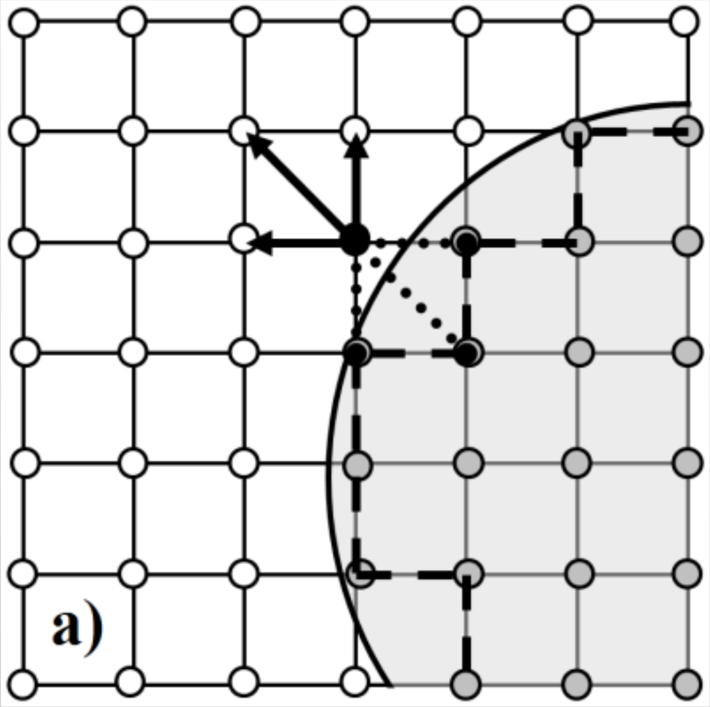
Eq. of state: $$p = \rho c_s^2$$

Viscosity: $$\nu = c_s^2 (\tau - \frac{\Delta t}{2})$$

The negative contribution (propagation viscosity) stems from second order expansion of the lattice streaming operator (see Succi's book)

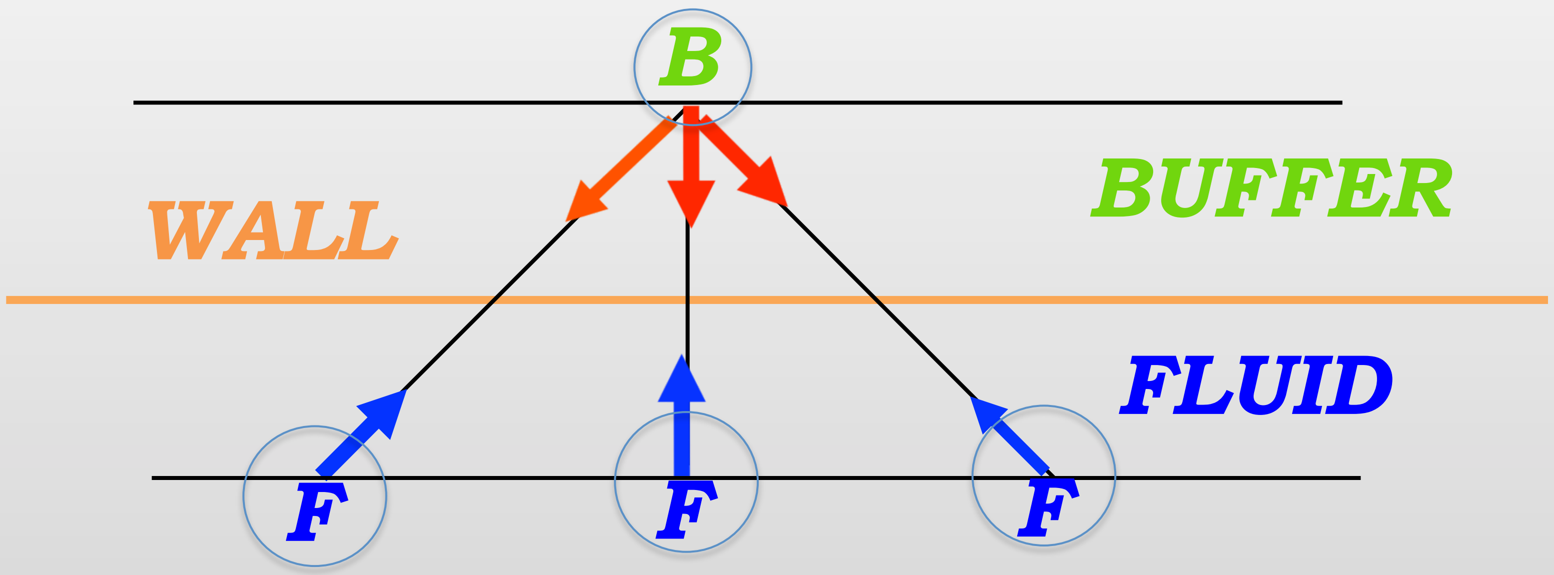
Boundary Conditions





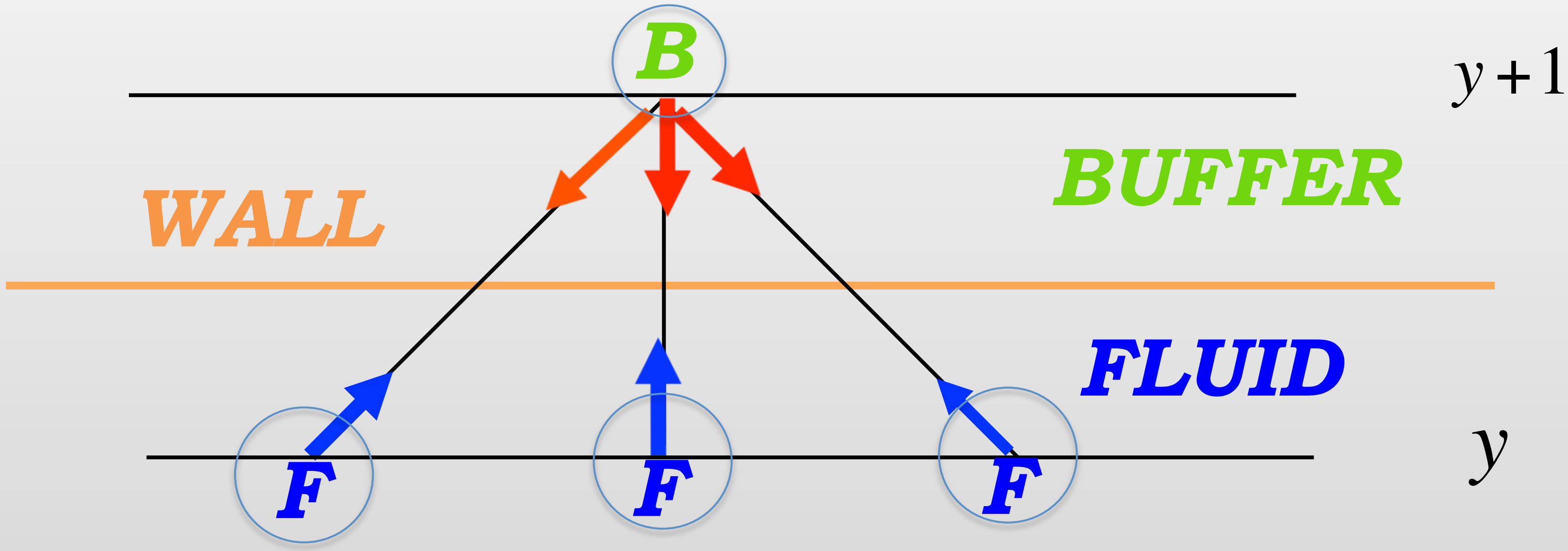
No-slip flow via bounce-back

$$f(W,t+1/2) = f_{in}(B,t) + f_{out}(F,t)$$



Bounce-Back

$$f(W,t+1/2) = f_{in}(B,t) + f_{out}(F,t)$$



$$f_{sw}(x,y+1) = f_{ne}(x-1,y)$$

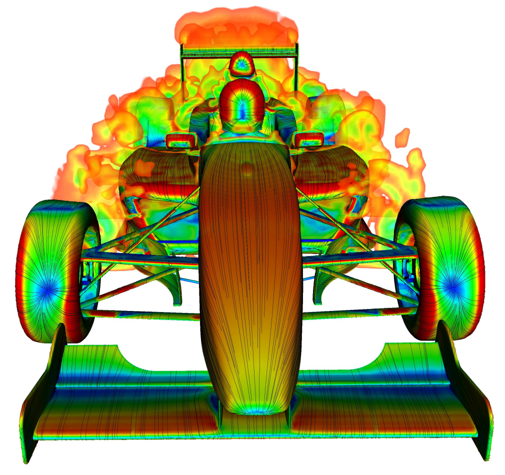
$$f_{s}(x,y+1) = f_{n}(x,y)$$

$$f_{se}(x,y+1) = f_{nw}(x+1,y)$$

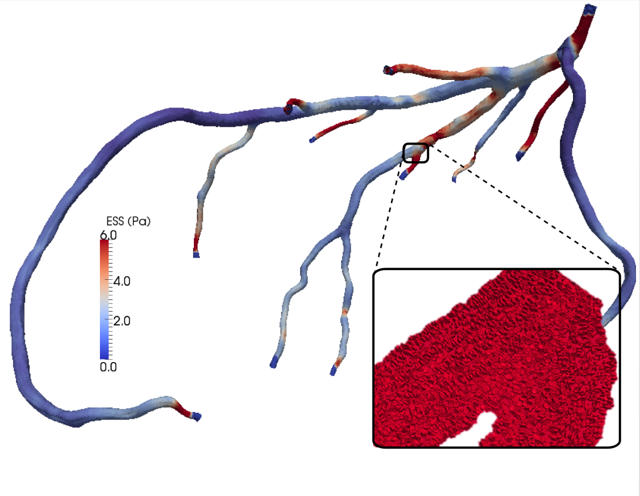
LBE assets

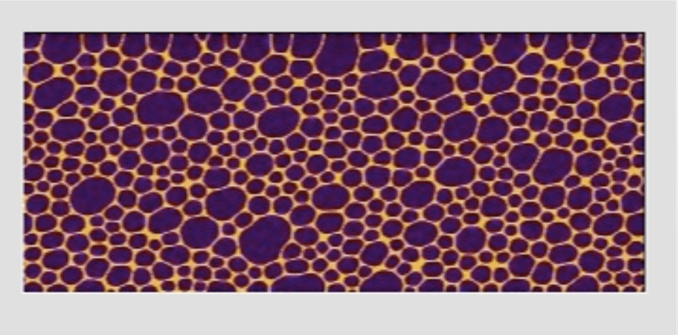
- Streaming is linear and exact (no $\vec{u}\cdot\vec{\nabla}\vec{u}$) $\vec{c}_i \cdot \nabla f$
- Non-linearity is local (round-off conservative)
  Laplacian-free dissipation
- Stress and pressure is local (weakly compressible)
- Easy handling of complex geometries (straight lines)
- Outstanding for parallel computing
- Emergent complexity nearly for free

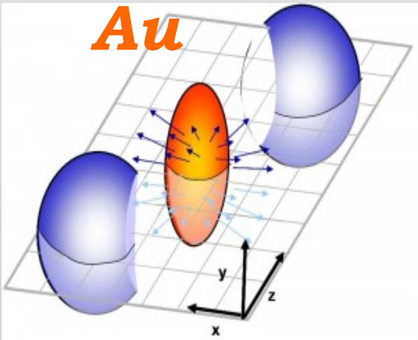
LB across scales: from turbulence to biopolymers to quark-gluon plasma

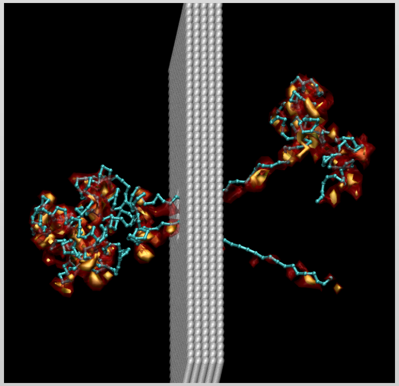


MOVIE time!!!









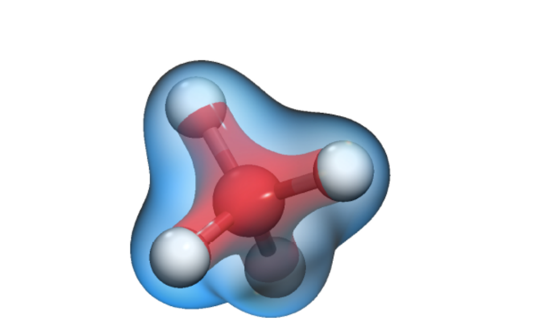


FIG. 1. Methane molecule, CH_4. The blue and red isosurfaces denote low and high electronic density, respectively. Using our model, we have obtained for the angles between bonds, 109.47 degrees, and a C-H bond distance of 108.6 pm.

Assignments

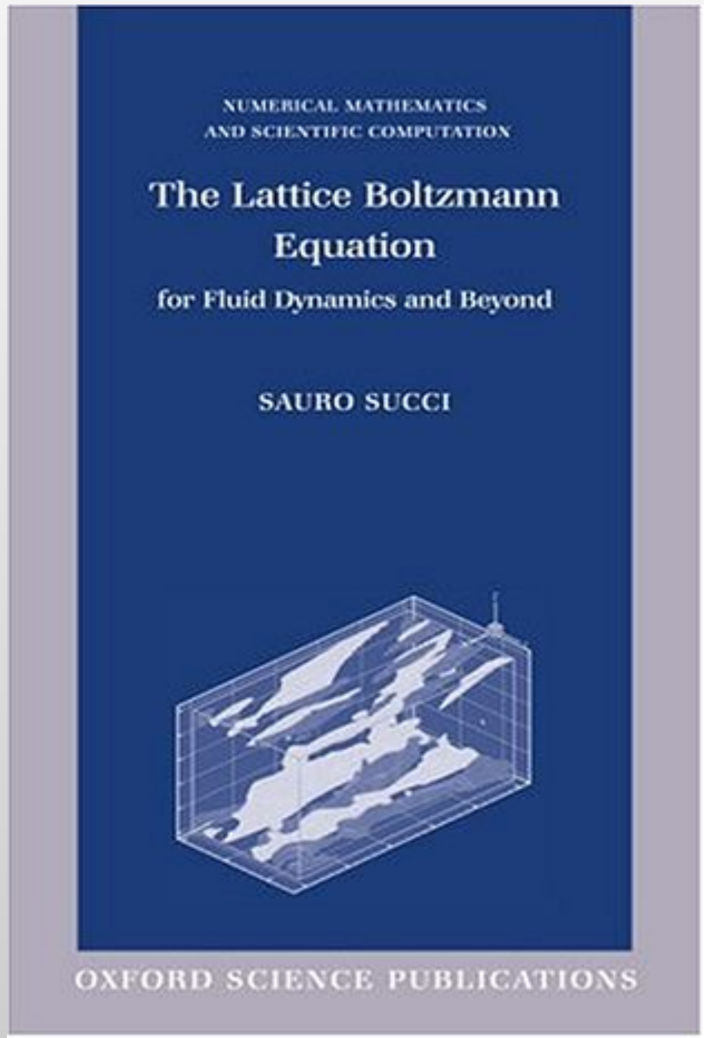
1. **Write a D2Q9 code for channel flow and run the Poiseuille flow at different viscosities (see lb2.f)**

2. **Same with a cylinder within the channel**

3. **Same with a random porous media**

Reference

(for the detail-thirsty, see my book! →



End of the lecture

Lattice vs continuum equilibria

Local **Global**

$$\mathrm{e}^{-\frac{1}{2}\left(\frac{\vec{v}-\vec{u}}{v_T}\right)^2} = e^{-\frac{v^2}{2v_T^2}} \sum_{n=0}^{\infty} H_n\left(\frac{\vec{v}}{v_T}\right)\left(\frac{\vec{u}}{v_T}\right)^n$$

Why not just take: $\vec{V} = \vec{c}_i$?

Galilean invariance requires infinite series in the Mach number
Infinite rank isotropic tensors, i.e. infinite connectivity!!!
Scaling invariance v/vthermal: global to local very hard