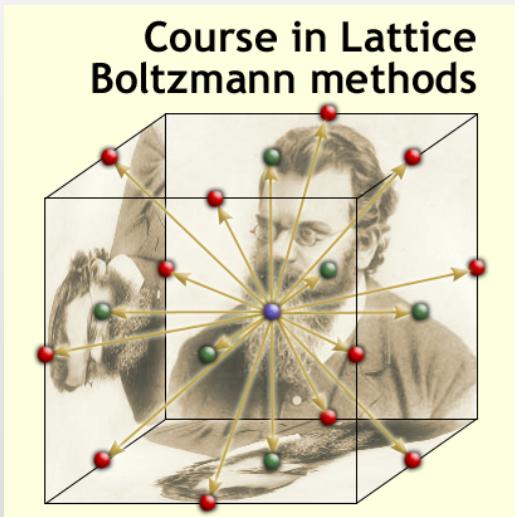


Lattice Boltzmann for multi-dimensional fluids



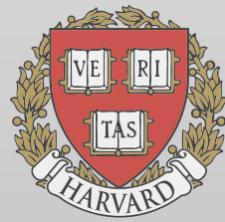
Sauro Succi

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 first 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)

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

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

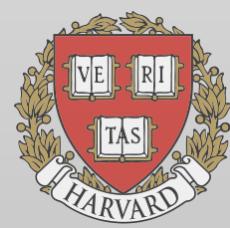
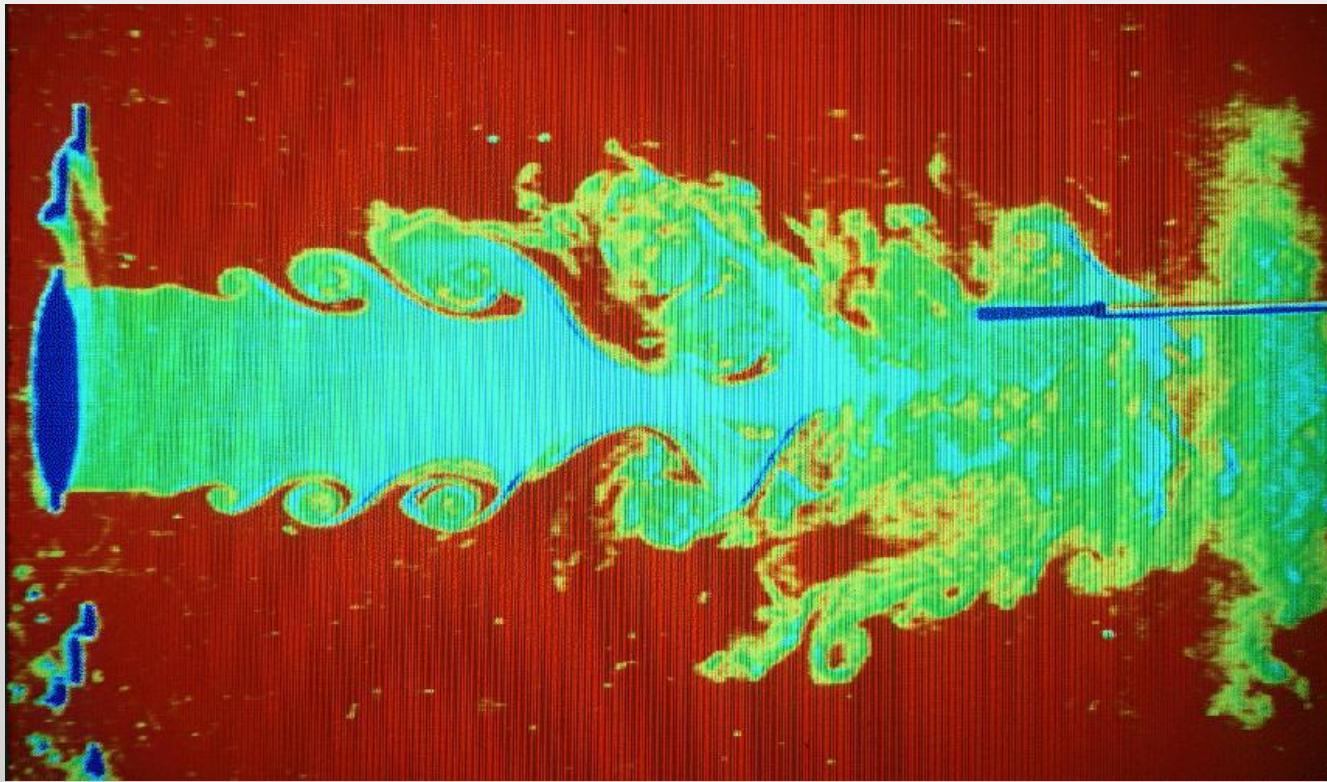
Reynolds number

$$\text{Re} = \frac{UL}{\nu}$$



Turbulence!

$\text{Re} \rightarrow \infty$

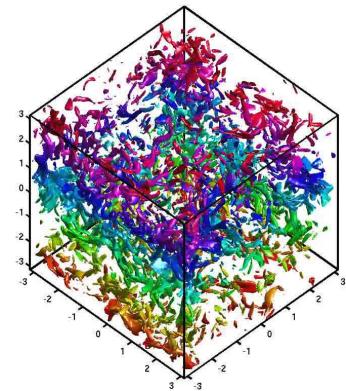


The scales of turbulence

- Kolmogorov length

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

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



Faucet, $\text{Re}=10^4$, $DOF=10^9$

Car/Airpl, $\text{Re}=10^6-8$, $DOF=10^{14-18}$

Geo/Astro, $\text{Re}=10^{10}$, $DOF=10^{22}$

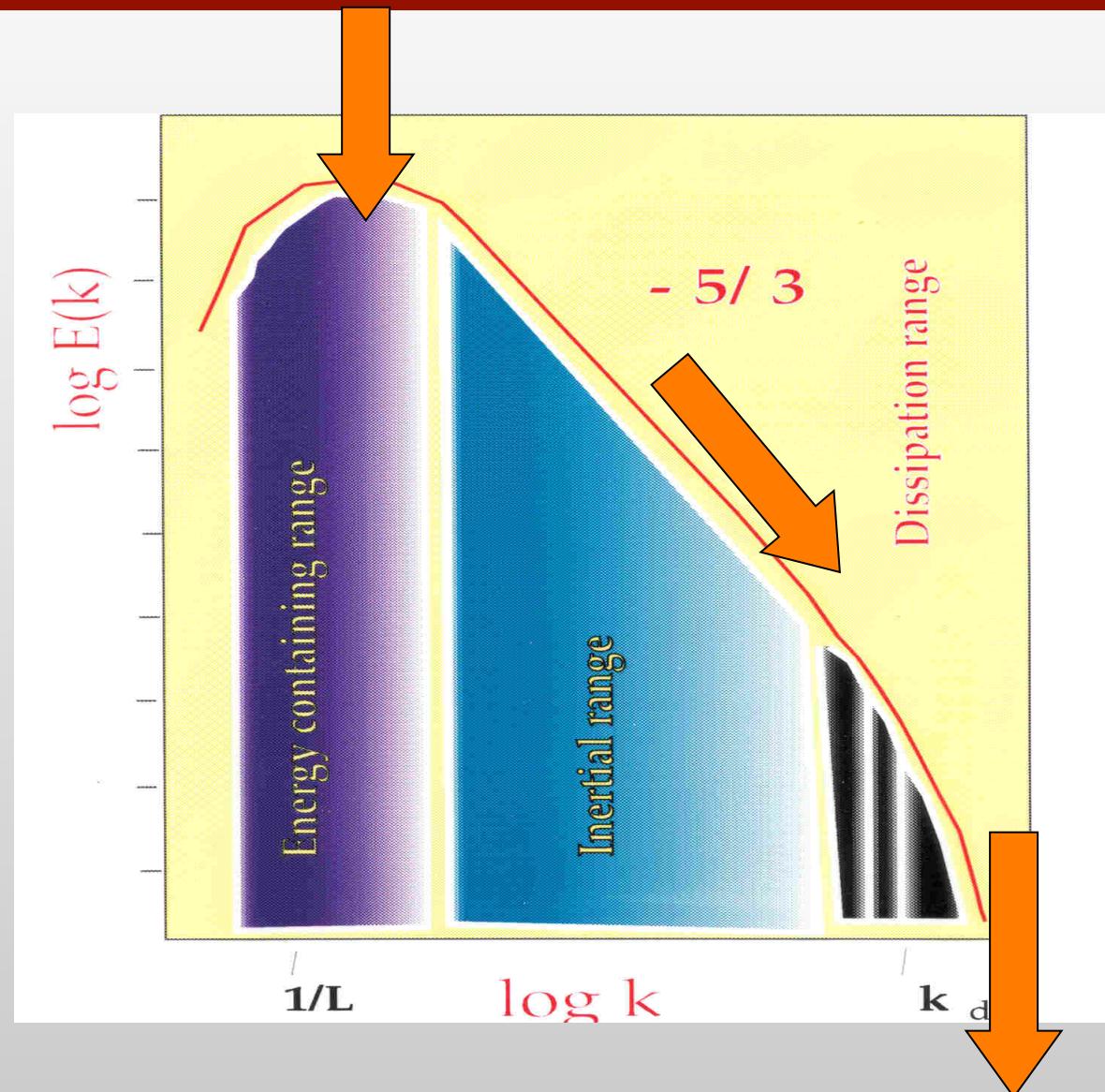
Energy spectrum: broad and gapless!

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 (Conservative form):

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

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

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

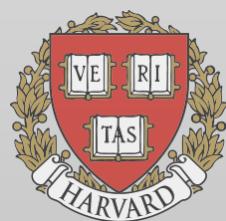
Advection

Pressure

Dissipation

of Macrofields= Constraints:

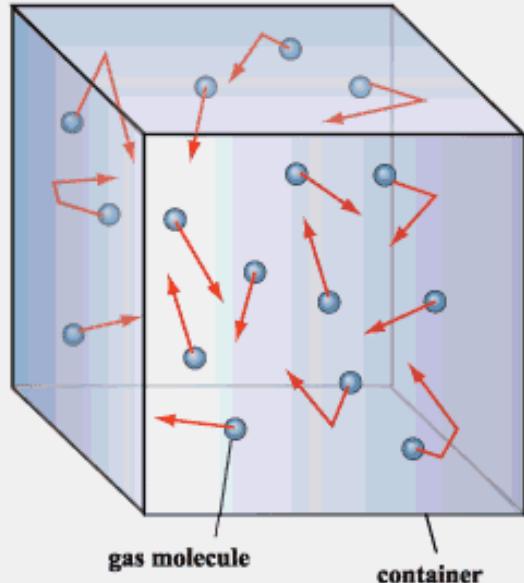
$$N_C = 1 + d + d(d+1)/2 = \{3, 6, 10\}$$



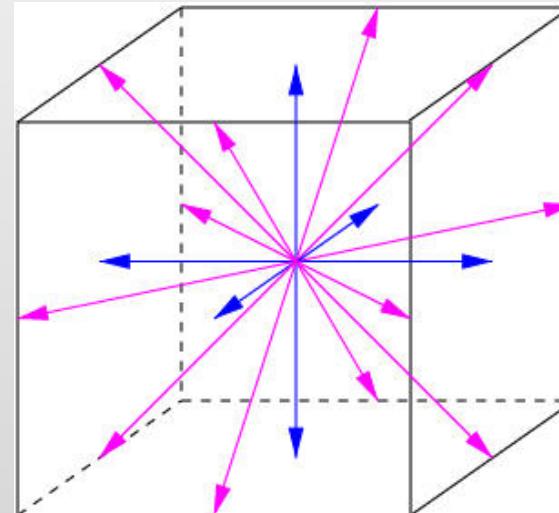
Lattice Boltzmann: Platonic hydrodynamics

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

Triple infinity to just 19!



Magic speeds!



Exact sampling of frequent events

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

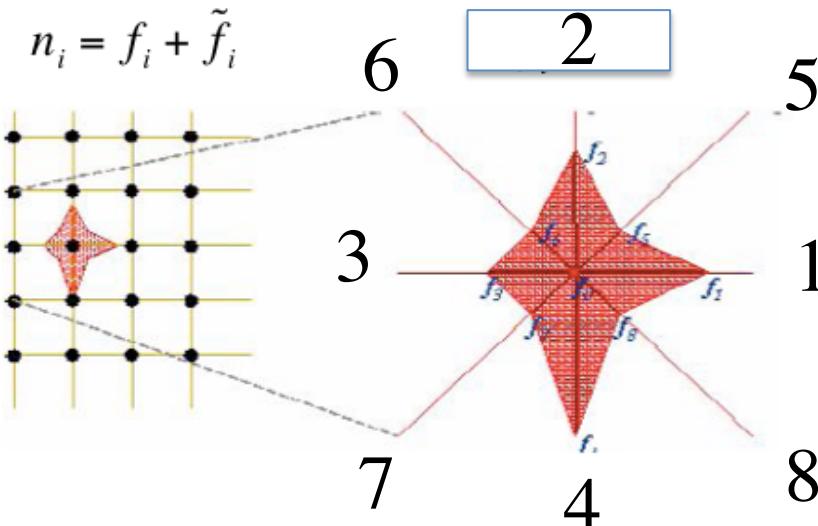
Lattice String Theory (?)

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 its shape (string dynamics).

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

The discrete-velocity distribution function

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

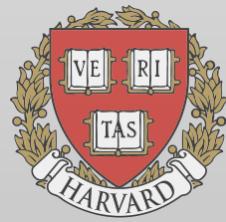


$$\vartheta_{\{1,2,3,4\}} = \{0, 1, 2, 3\}\pi / 2$$

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

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

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



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:

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

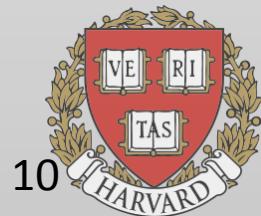
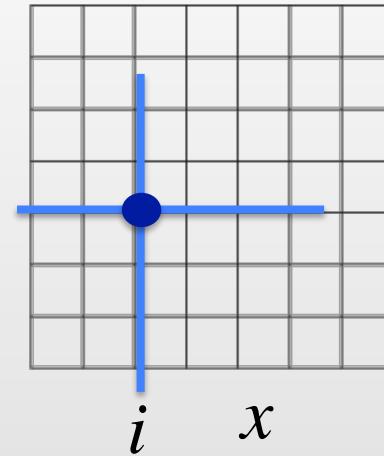
In $d+d$ dimensions: $DoF = N^{2d}$

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

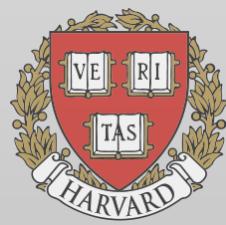
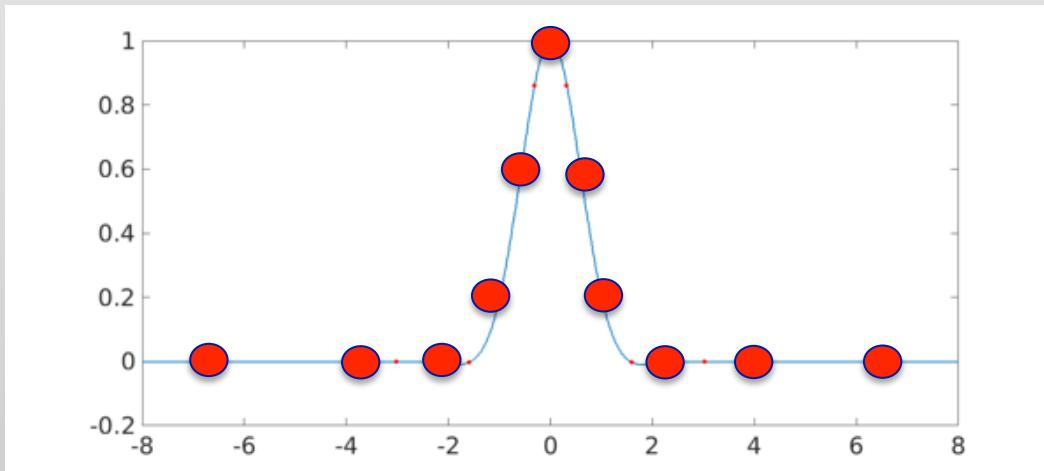


Sampling versus discretization

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

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

$$i = 0, 2d < b < 3^d$$

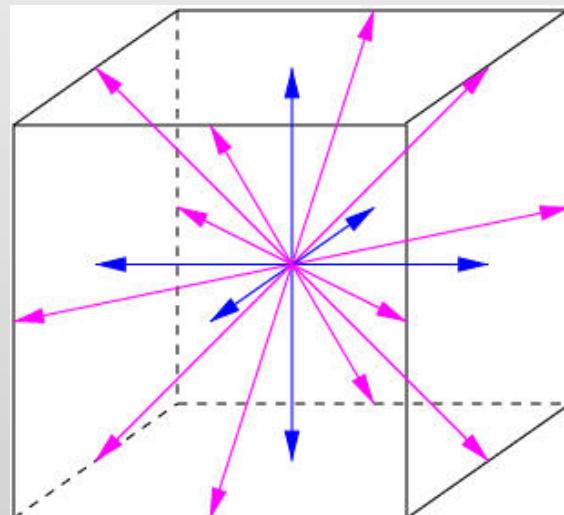
How to find:

c_i, Omega_ij , f_i^eq
In d-dimensions?

Lattice BGK (single-time relaxation)

$$\Omega_{ij} = \Omega \delta_{ij}$$

$$\omega = \Omega \Delta t = \Delta t / \tau$$

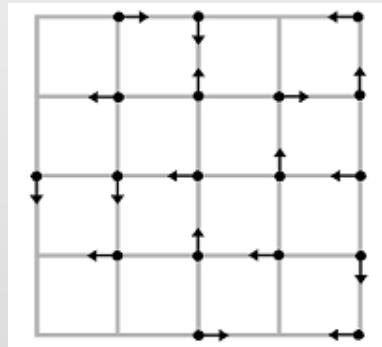


$$(\Delta \vec{r}_i = \vec{c}_i \Delta t)$$

Navier-Stokes in $d=2$ dimensions

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

D2Q4=HPP (1976)



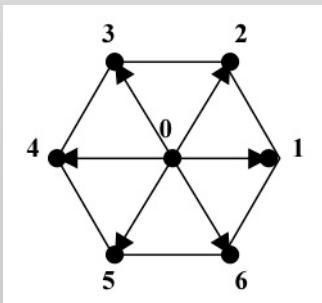
$$\vec{c}_1 = (1, 0) \quad \vec{c}_2 = (0, 1)$$

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

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

Natural: 4 speeds versus 6 macrofields: no way!

D2Q6=FHP (1986)

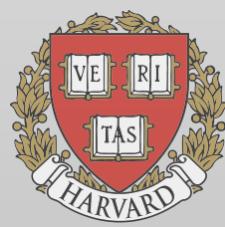
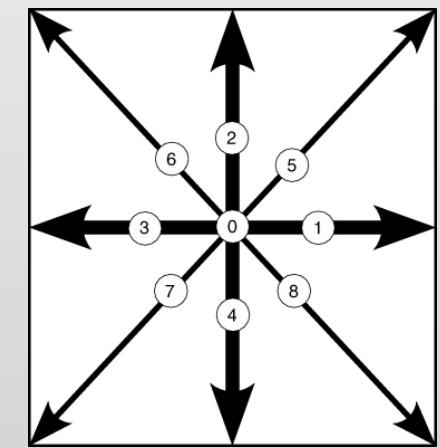


$$c_{ix} c_{iy} \neq 0 \Rightarrow u_a u_b \neq 0 \quad \text{YES!}$$

Natural: 6 speeds versus 6 macrofields: ok!

But 9 is better (D2Q9)

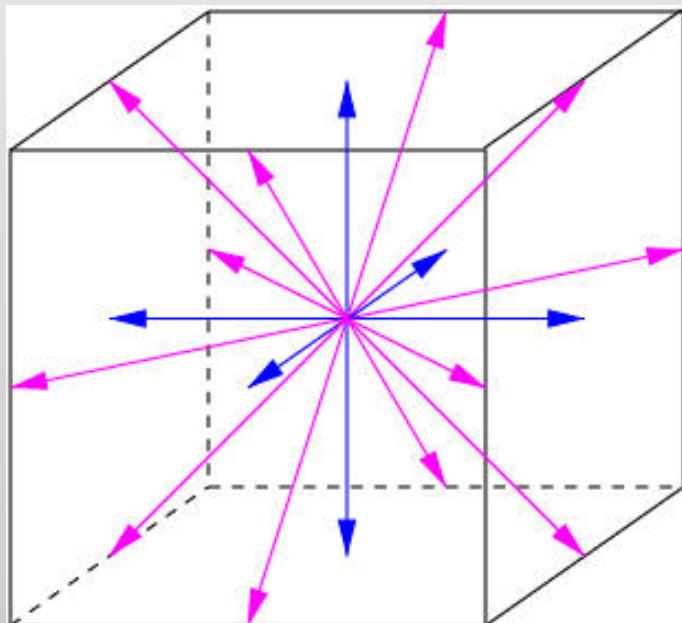
D2Q9 (1989)



Navier-Stokes in d=3 dimensions

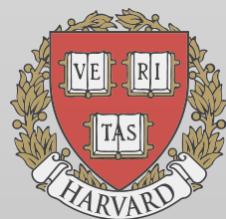
$$Hydro = \{\rho; u_x, u_y, u_z; P_{xx}, P_{xy}, P_{xz}, P_{yy}, P_{yz}, P_{zz}\}$$

$$f_i = \{Vx = \pm c; Vy = \pm c, Vz = \pm c\} \quad \text{6 speeds vs 10 fields: NO WAY!}$$



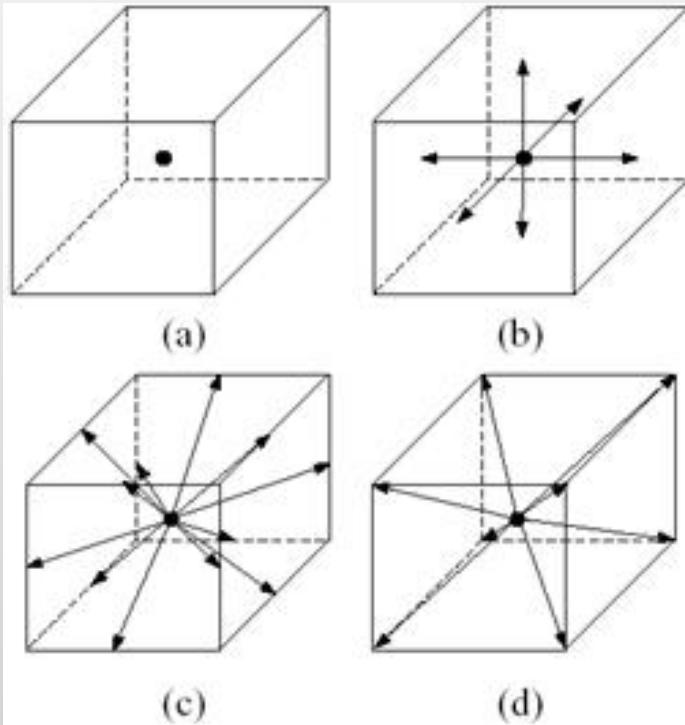
D3Q19: YES!
10 hydrofields + 9 “ghosts”

D3Q27: yes, of course

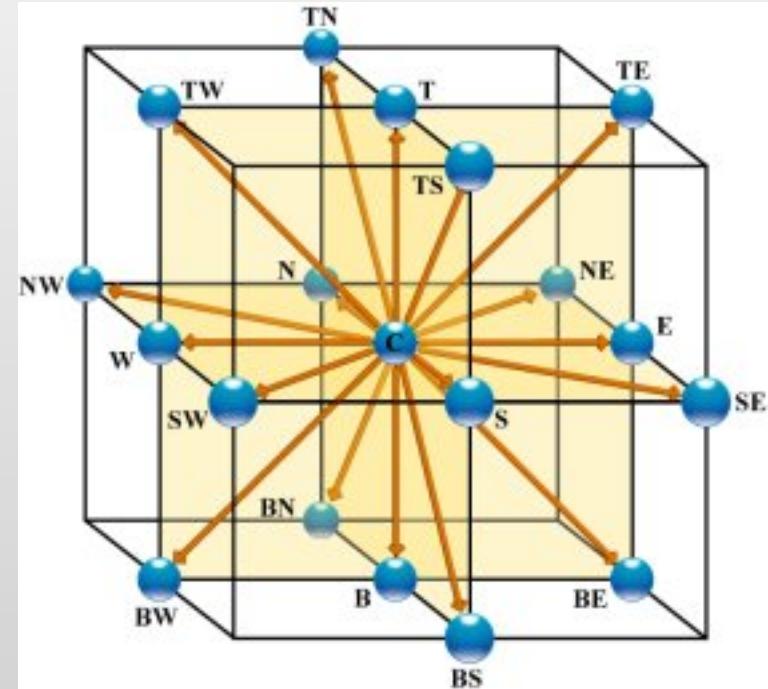


Standard 3d LB lattices

D3Q27=(D1Q3) 3

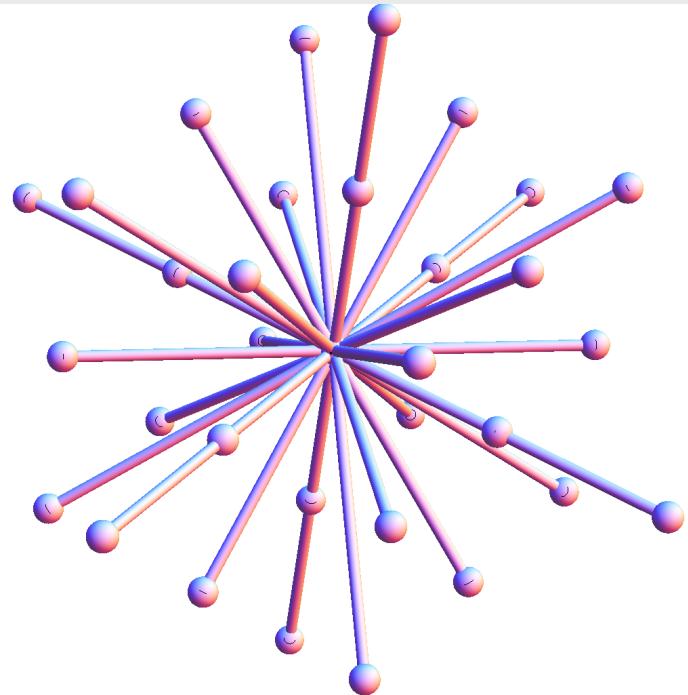


D3Q19= D3Q27-8 vertices

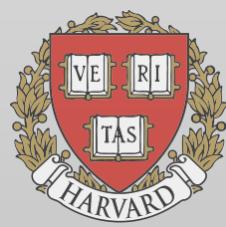
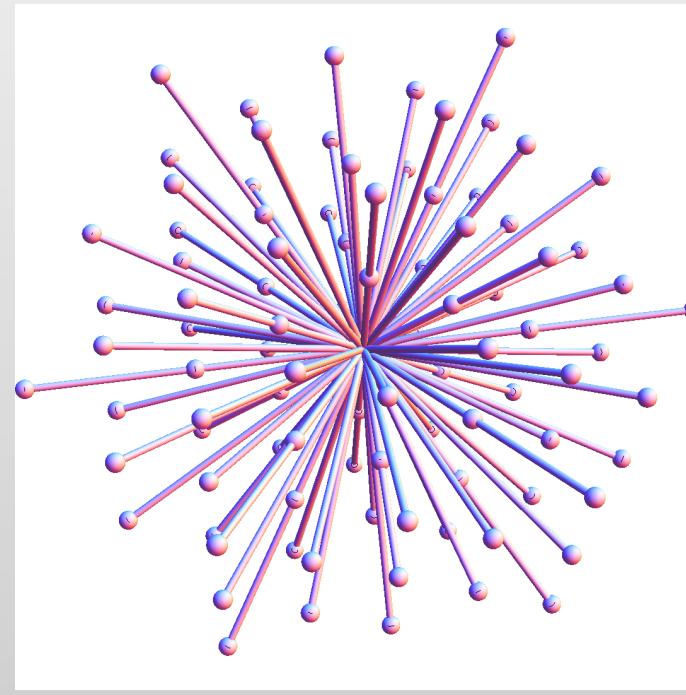


Higher order lattices

D3Q39: order 6 isotropy

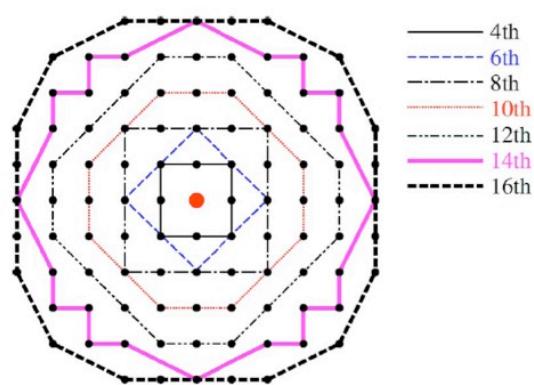


D3Q93: order 8 isotropy

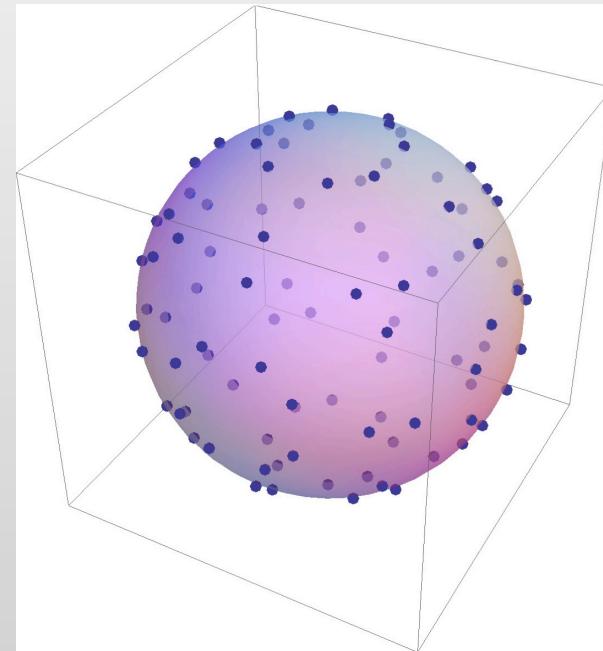


Very Higher Order Lattices

D=2, up to order 16!



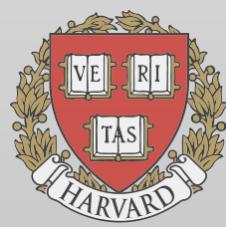
D=3, relativistic



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:

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

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

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

By imposing:

$$\rho^{eq} = \rho$$

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

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

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:

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

$$\partial_t (\rho u_a) + \partial_b P_{ab} = -\Omega (J_a - J_a^{eq}) \quad \sum_{i=0}^b f_i c_{ia} = J_a \equiv \rho u_a$$

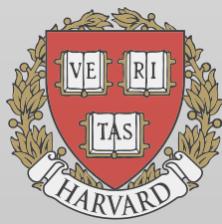
By imposing:

$$J_a^{eq} = J_a$$

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

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

Is it Navier-Stokes? NOT YET! Constraints must be imposed on P_{ab}



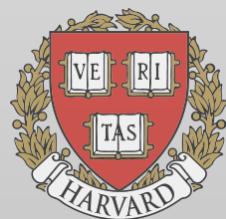
Moment matching: momentum

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:

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

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

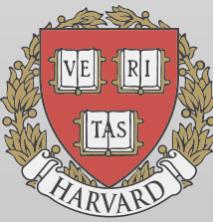
Now $P_{ab} \neq P_{ab}^{eq}$ because momflux is **not** a micro-invariant!

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

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

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

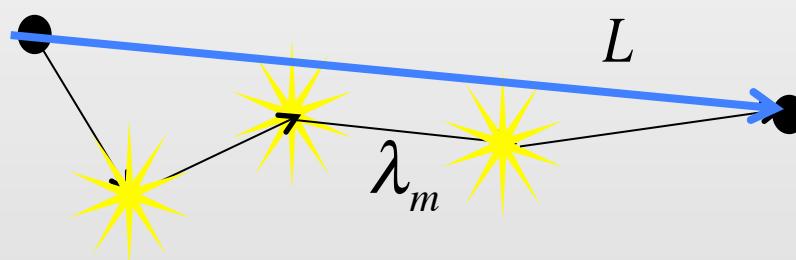
How do we close this equation?



Boltzmann to Navier-Stokes

1. Scale separation:

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



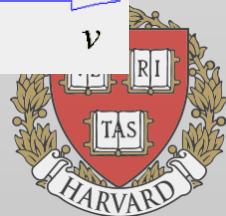
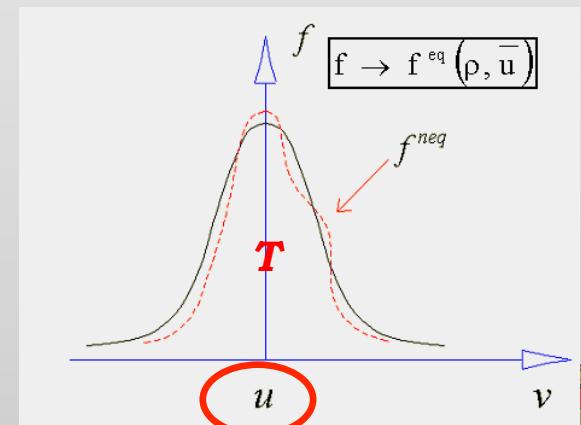
$$Kn = \frac{\lambda_m}{L} \ll 1$$

2. Weak departure from local equilibrium:

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

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

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



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 $\tau = 1/\Omega$:

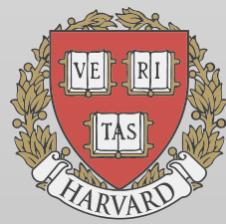
$$P_{ab} \approx P_{ab}^{eq} - \tau \partial_c Q_{abc}$$

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

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



Inertia+Pressure



Momflux: enslaving

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

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

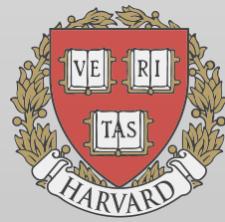
This must now match exactly the Navier-Stokes equations:

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

Which implies the following **tensorial** constraints:

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

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



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

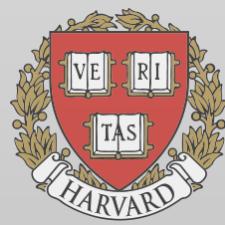
$$P_{ab}^{eq} \equiv \sum_{i=0}^b f_i^{eq} c_{ia} c_{ib} = \rho u_a u_b + p \delta_{ab}$$

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

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

Mass

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

Momentum

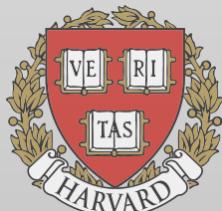
$$\sum_{i=0}^b w_i c_{ia} c_{ib} = c_s^2 \delta_{ab}$$

Pressure

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

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

Advection-Dissipation



Lattice Equilibria

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

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

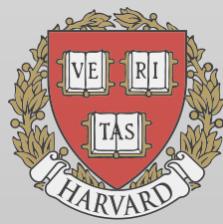
where:

$$u_i = \frac{c_{ia} u_a}{c_s^2} = \frac{\vec{u} \cdot \vec{c}_i}{c_s^2}$$
 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 $(\sum_i Q_{iab} = \sum_i c_{ia} c_{ib} - c_s^2 \delta_{ab} = 0)$

Question: How do we find the optimal weights?



Lattice Equilibria

By inserting

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

in the list of hydrodynamic constraints, we obtain:

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

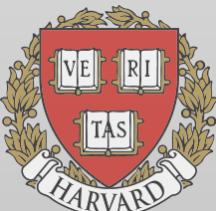
0th order isotropy

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

2nd order isotropy

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

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:

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

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

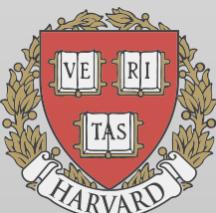
Order 0: Normalization

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

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

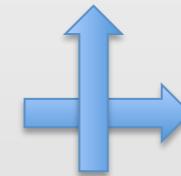
Expand the local Maxwell-Boltzmann to third order in Mach number:

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

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

Dipole

$$u_a$$



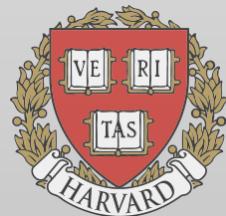
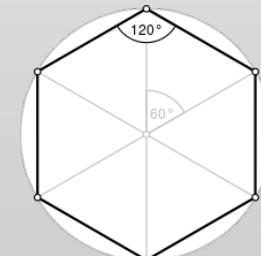
$$q_i = \frac{Q_{iab} u_a u_b}{c_s^4}$$

Quadrupole $u_a u_b$

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

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

Hexapole:



D1 lattice equilibria

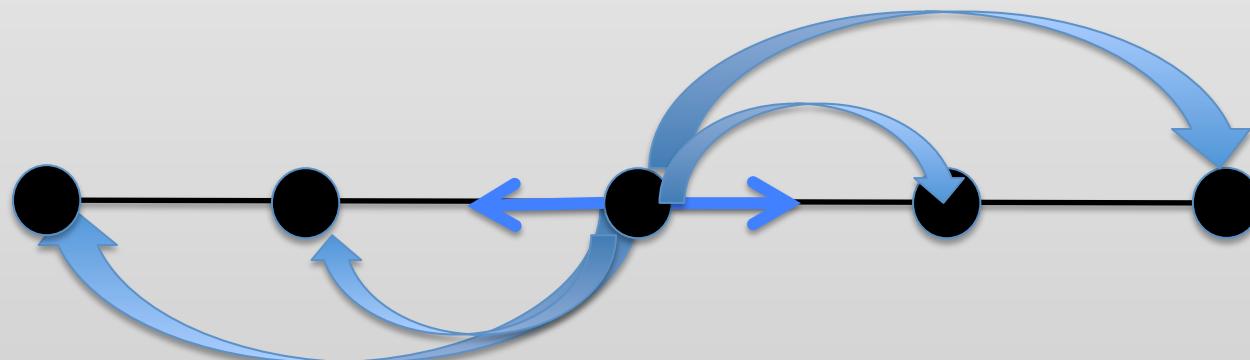


D1Q3

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

$$w_i = \frac{1}{6} \{1, 4, 1\}$$

$$c_s^2 = 1/3$$



D1Q5

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

Compute D2Q9 equilibria

$$u_0 = 0$$

Linear (Dipole)

$$c_s^2 = 1/3$$

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

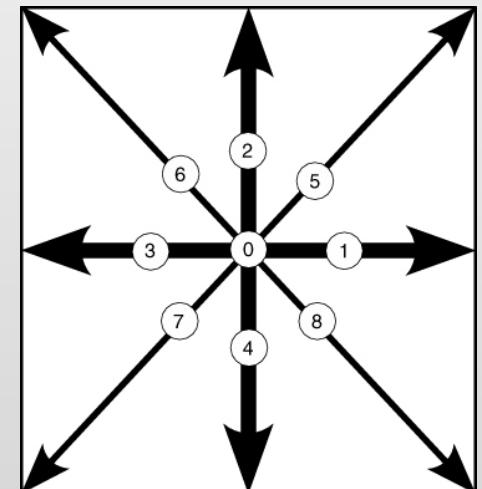
$$u_5 = +3(u_x + u_y) \quad u_6 = +3(-u_x + u_y)$$

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

Quadratic (quadrupole)

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

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



D2Q9 equilibria

$$w_i = \left\{ \frac{4}{9}; \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}; \frac{1}{36}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36} \right\} \quad c_s^2 = 1/3$$

Quadratic polynomials (Check the algebra!):

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

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

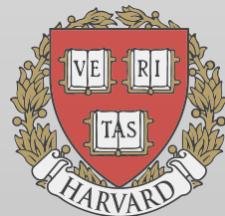
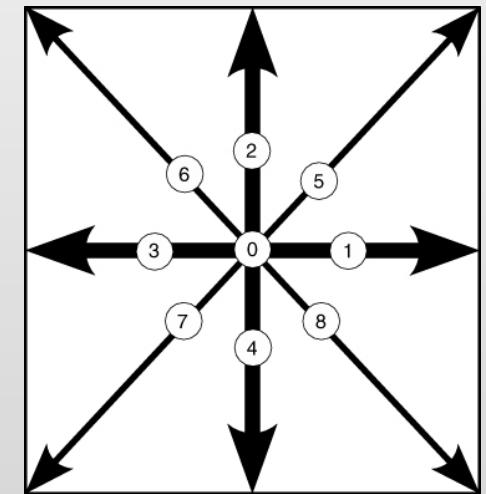
$$f_3^{eq} = \frac{\rho}{9} (1 - 3u_x + 3u_x^2)$$

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

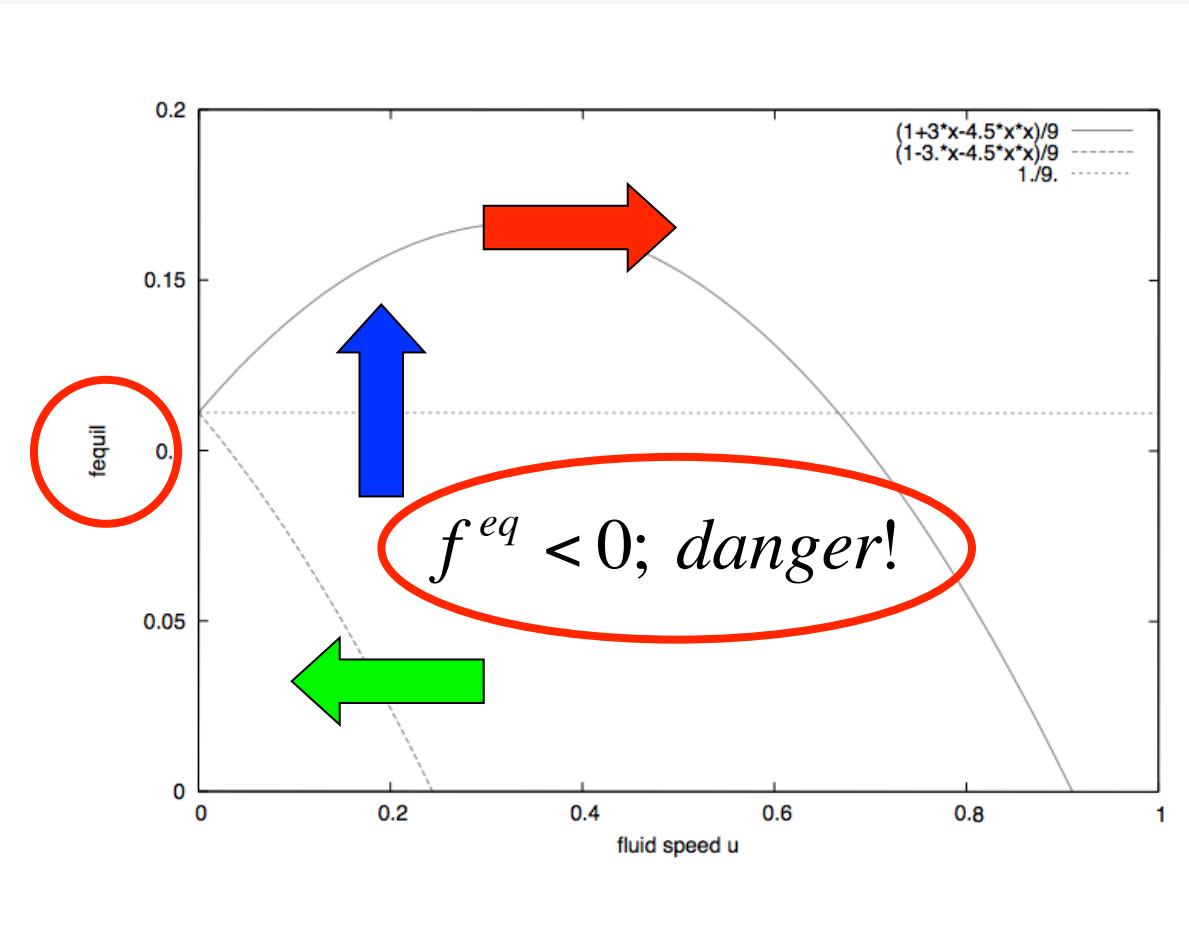
$$f_4^{eq} = \frac{\rho}{9} (1 - 3u_y + 3u_y^2)$$

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

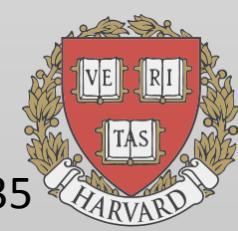
$$f_7^{eq} = \frac{\rho}{36} (1 - 3u_x - 3u_y + 2u_x u_y) \quad f_8^{eq} = \frac{\rho}{36} (1 + 3u_x - 3u_y - 2u_x u_y)$$



Realizability (positivity): Low Mach



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



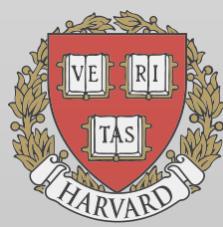
Summary

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: $p = \rho c_s^2$

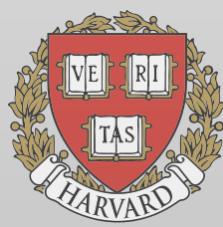
Viscosity: $\nu = c_s^2 (\tau - \frac{\Delta t}{2})$

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

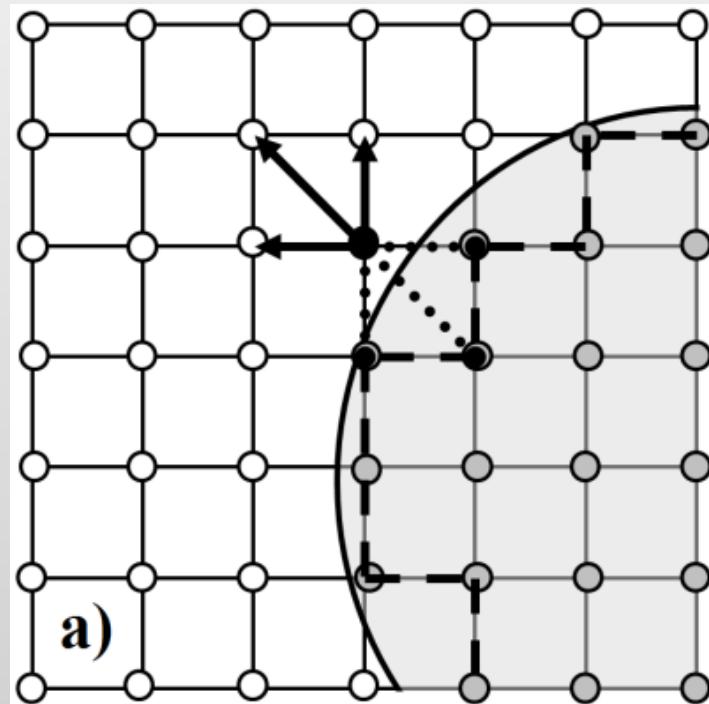
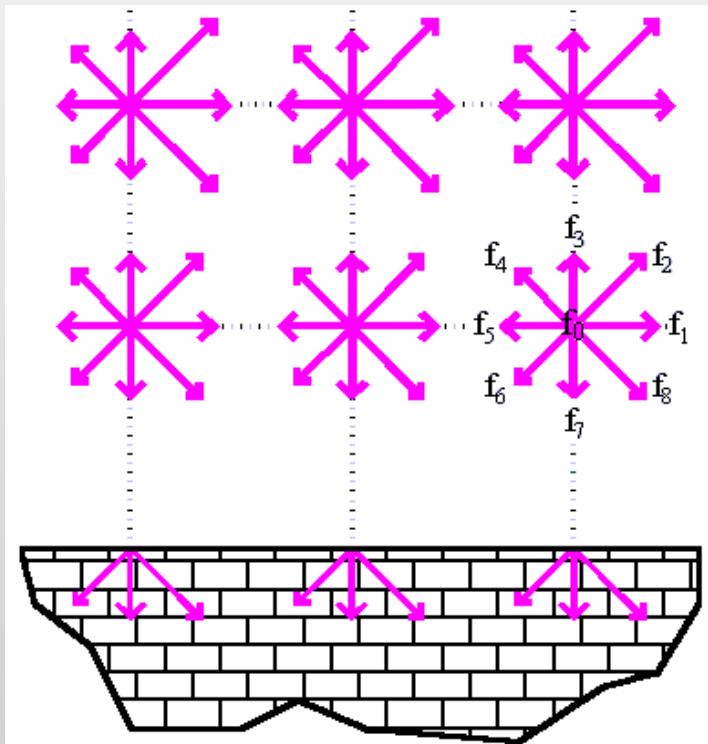


LBE assets

- + *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*

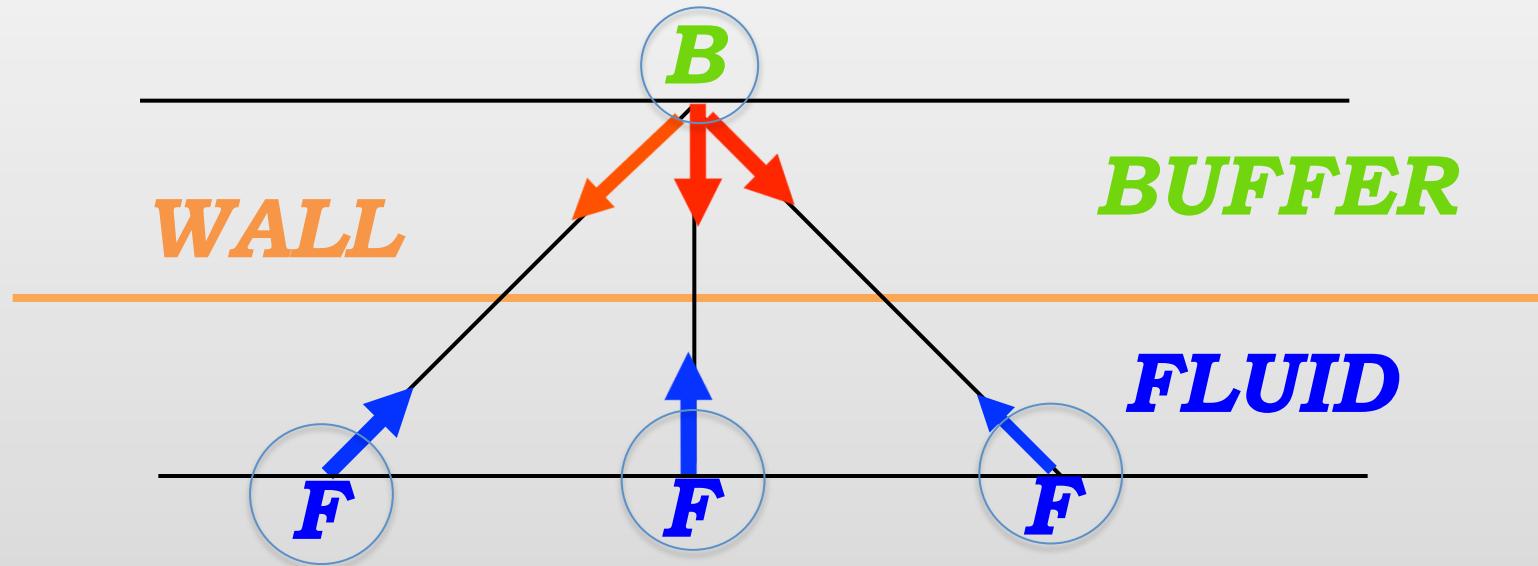


Boundary Conditions



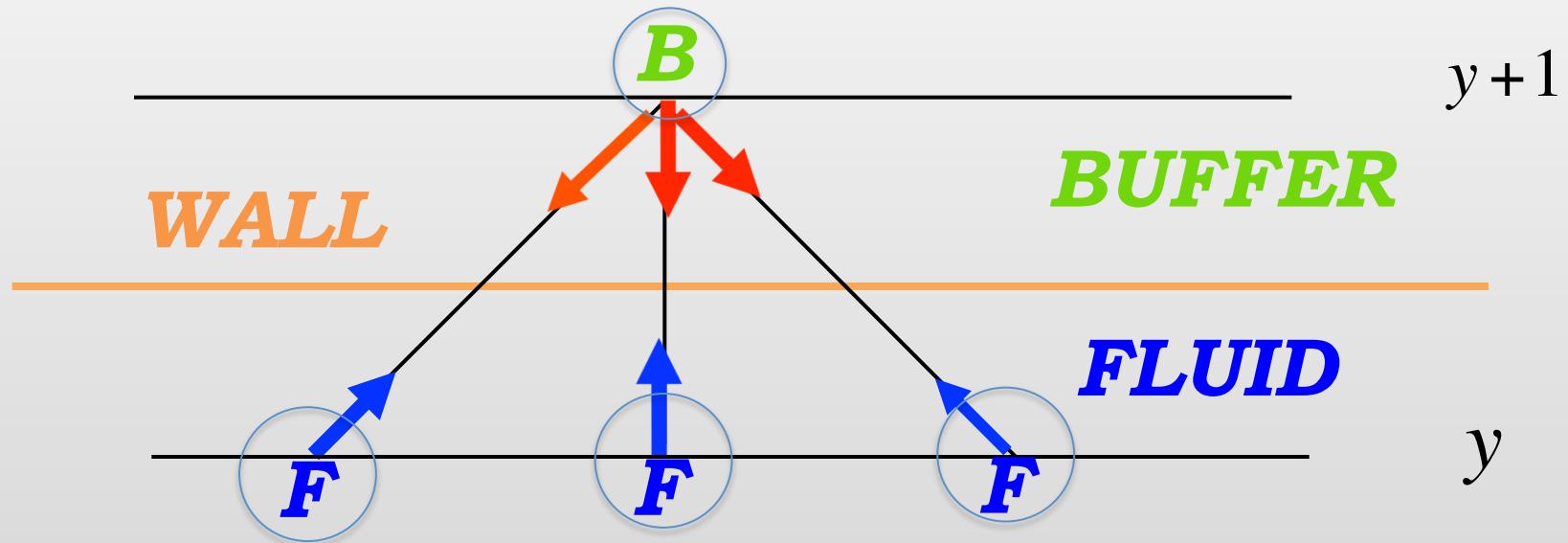
No-slip flow via bounce-back

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



Bounce-Back

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



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

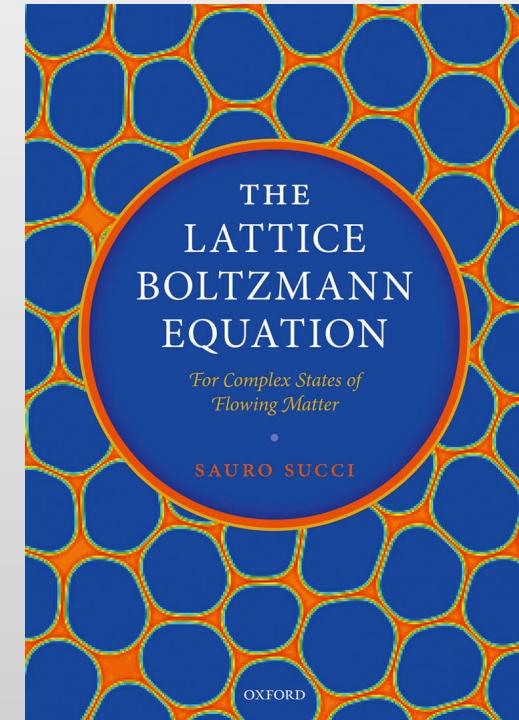
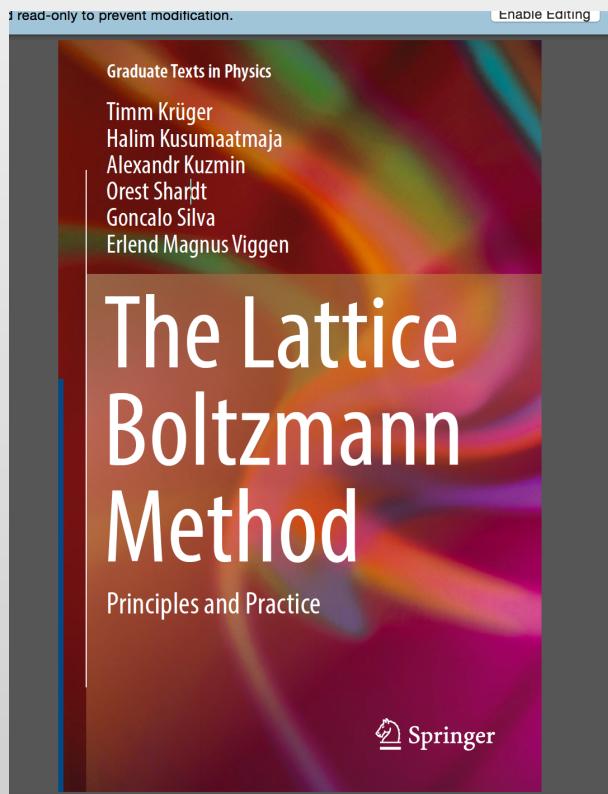
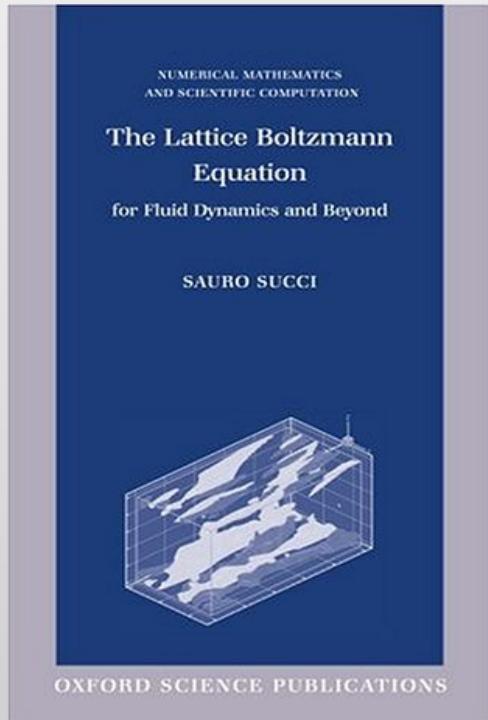
$$f_s(x, y+1) = f_n(x, y)$$

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

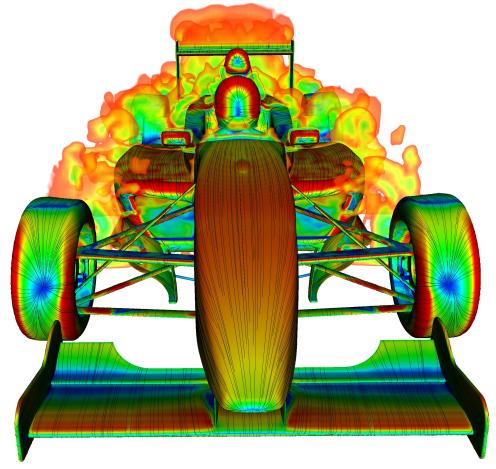
References

End of Lecture

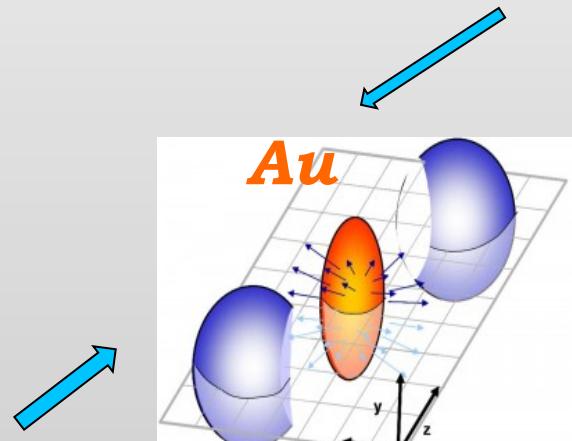
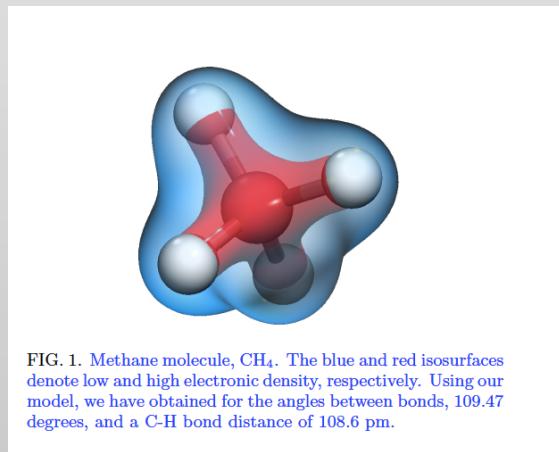
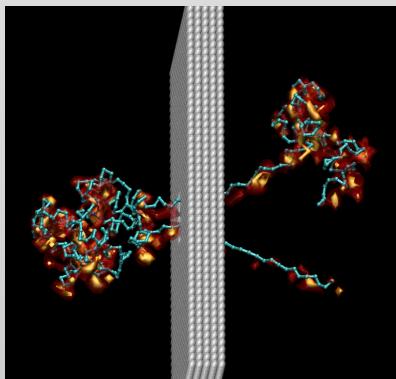
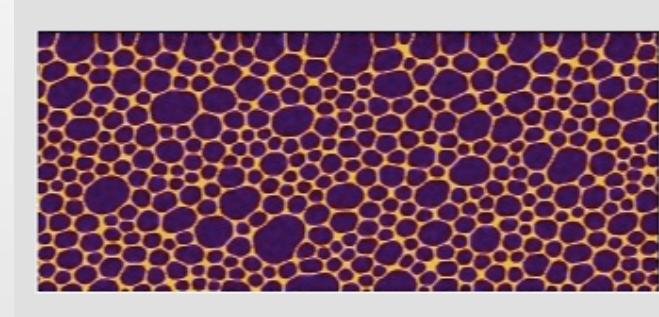
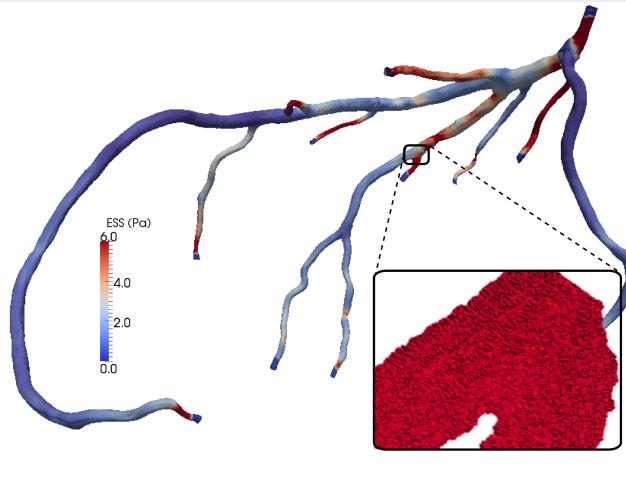
(for the detail-thirsty, see these books!)



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

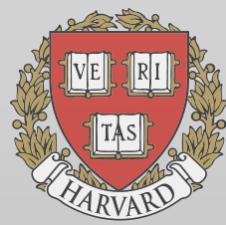


MOVIE time!!!

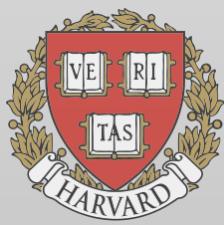


Assignments

- 1. Write a D2Q9 code for channel flow and run the Poiseuille flow at different viscosities (see Ib2.f)**
- 2. Same with a cylinder within the channel**
- 3. Same with a random porous media**



End of the lecture



Lattice vs continuum equilibria

$$\begin{array}{ccc} \text{\color{red} Local} & & \text{\color{red} Global} \\ e^{-\frac{1}{2}\left(\frac{\vec{v}-\vec{u}}{v_T}\right)^2} & = & e^{-\frac{v^2}{2v_T^2}} \sum_{n=0}^{\infty} H_n\left(\frac{\vec{v}}{v_T}\right)\left(\frac{\vec{u}}{v_T}\right)^n \end{array}$$

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/v_{thermal} : global to local very hard

