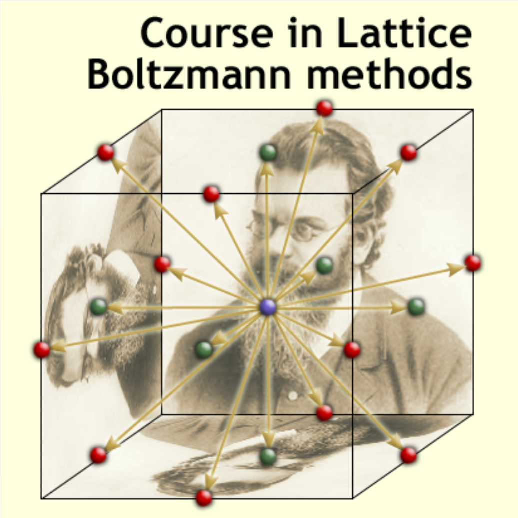
Lattice Boltzmann: Introduction



Sauro Succi

Boltzmann Kinetic Theory

Ludwig Boltzmann (1844-1906)

The man who trusted atoms …

Statistical Physics

Four basic levels:


MACRO

Continuum Fields

$$\partial_t u + (u \cdot \nabla) u = -\frac{\nabla P}{\rho} + \nu \Delta u$$

MESO

Probability distribution functions

$$\partial_t f + (v \cdot \nabla) f = -\frac{1}{\tau}(f - f^{(eq)})$$

MICRO

Particles

$$\frac{d^2 r_i}{dt^2} = -\sum_{j>i} \nabla V_{ij}$$

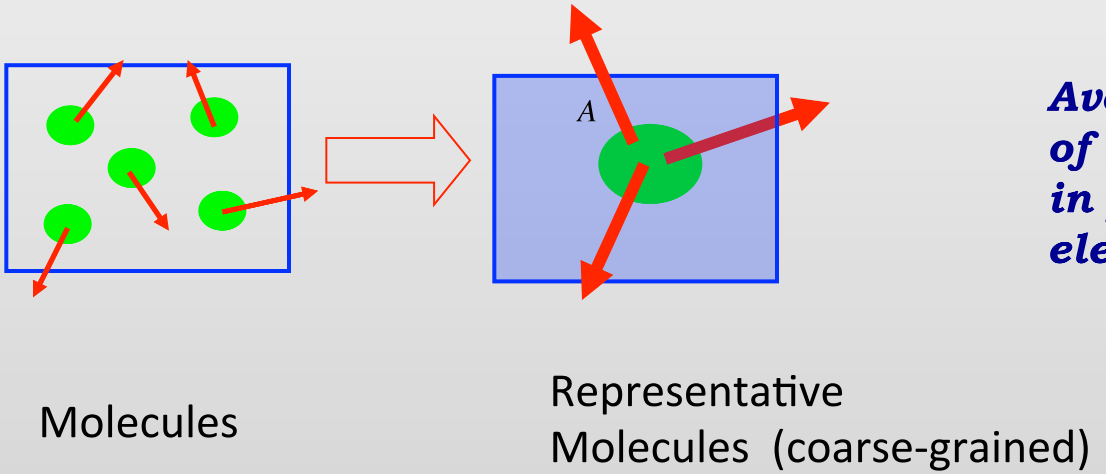
QUANTUM

Complex Quantum Fields

$$i\hbar \partial_t \Psi = H \psi$$

Boltzmann: Probability Distribution Function

$$\boxed{\Delta N = f(\vec{r}, \vec{p}; t)\Delta\vec{r}\Delta\vec{p}}$$



Average number of molecules in phase-space element dr*dp

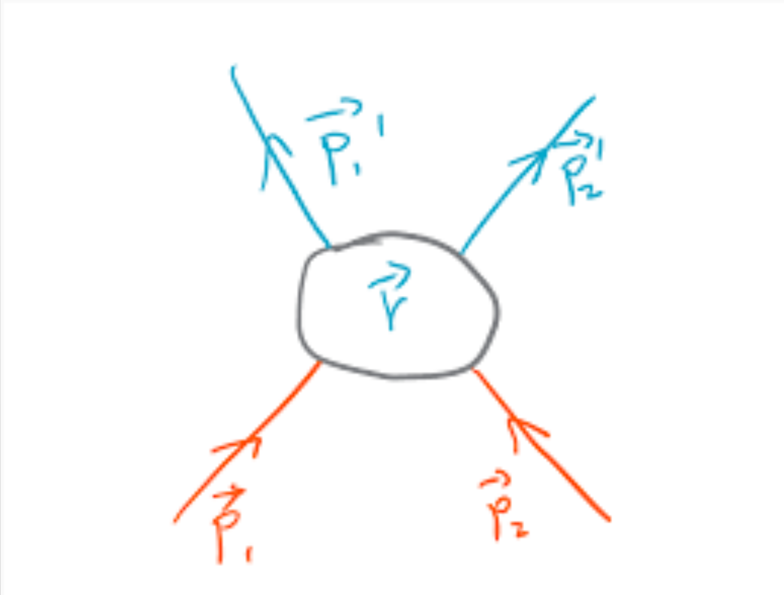
f lives in a 6-dimensional world: phase-space

The Boltzmann kinetic equation

$$\underbrace{\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}}}_{\text{Streaming:}} = Q[f,f] = Q^{+} - Q^{-}$$

Collisions

A continuity Eq. In 6-dim Phase space+ collision source



Binary collisions take particles IN (Q+) and OUT (Q-) of the phase Space element **dr*dp**

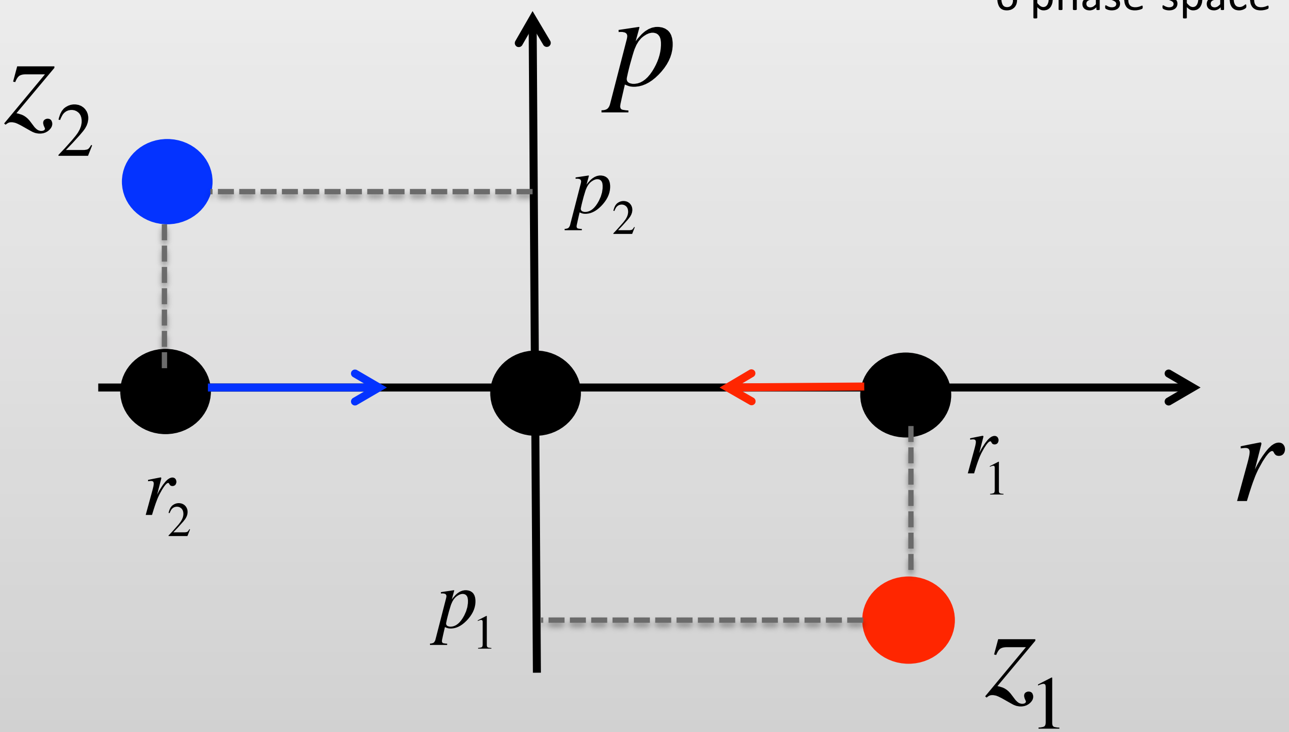
Phase-Space representation

$$z = \{\vec{r}, \vec{p}\}$$

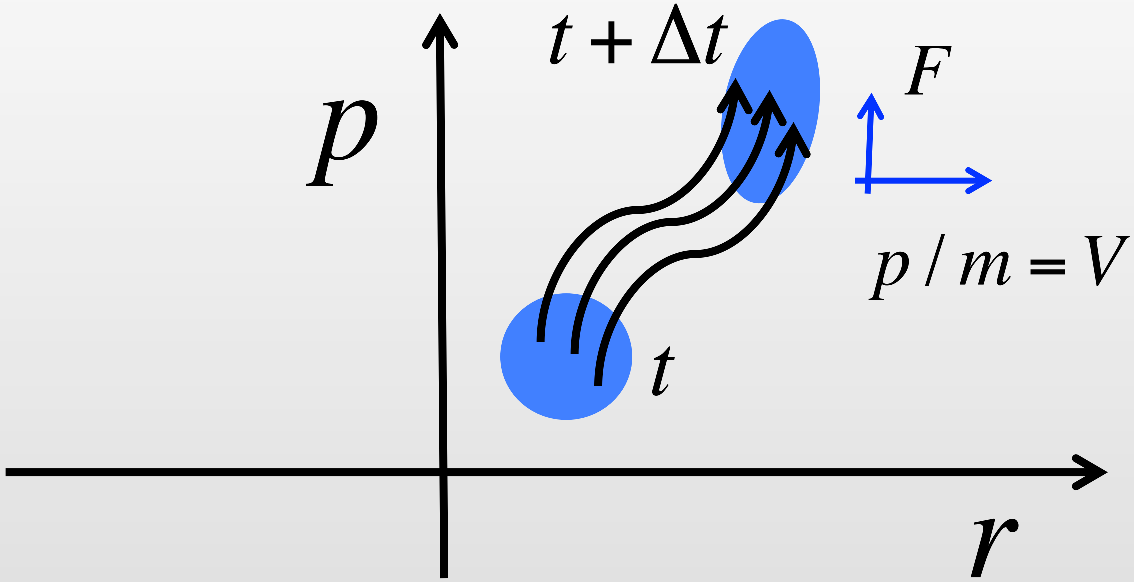
3 space coordinates **r**

3 momentum **p**

6 phase-space **z**



Phase-Space Fluid: Liouville theorem



$$\begin{cases} \dot{r} = p/m \\ \dot{p} = F \end{cases}$$

Phase-space volume is conserved under motion:

$$|\delta r(t)\delta p(t)| = |\delta r(t+\delta t)\delta p(t+\delta t)|$$

Since the number is conserved, the distribution also is:

$$\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + \frac{p}{m}\frac{\partial f}{\partial r} + F(r)\frac{\partial f}{\partial p} = 0$$

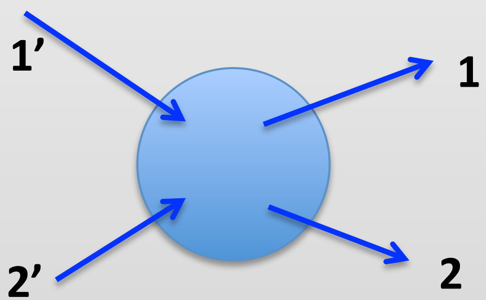
Collisions act as a source/sink in momentum space p but they are completely local in configuration space r

Collisions

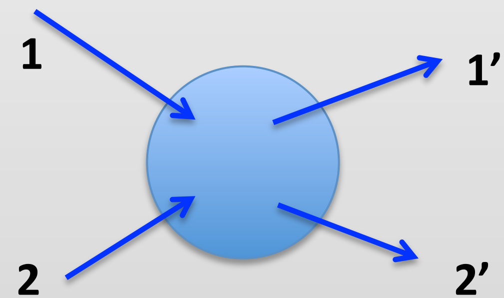
$$Q = \int [f(\vec{p}\,'_1)f(\vec{p}\,'_2) - f(\vec{p}_1)f(\vec{p}_2)]P(\vec{p}_1,\vec{p}_2 \rightarrow \vec{p}\,'_1,\vec{p}\,'_2)d\vec{p}_2 d\vec{p}\,'_1\, d\vec{p}\,'_2$$

The transition probability contains the molecular details

Gain



Loss



The interaction range **R** goes to zero. Collisions are complicated but **LOCAL in space**

Conservation laws

MASS $m_1 + m_2 = m'_1 + m'_2$

MOM $\vec{p}_1 + \vec{p}_2 = \vec{p}\,'_1 + \vec{p}\,'_2$

ENE $p_1^2/2m_1 + p_1^2/2m_2 = p'^2_1/2m_1 + p'^2_2/2m_2$

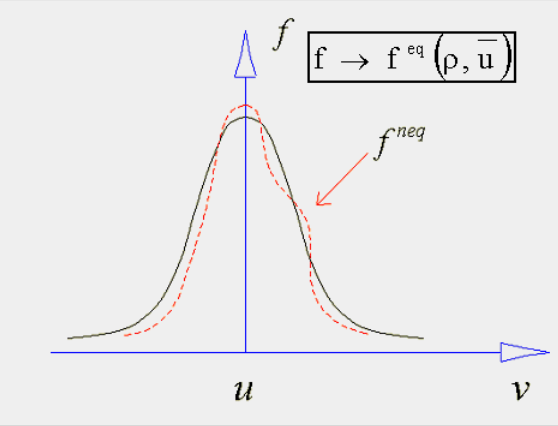
Local equilibrium (dynamic)

Gain=Loss

$$\boxed{Q^+ = Q^- \Leftrightarrow Q = 0}$$

Maxwell-Boltzmann local equils:

$$\boxed{f^{eq} = \frac{\rho}{(2\pi V_{th}^2)^{D/2}} e^{-(V-u)^2/2V_{th}^2}}$$

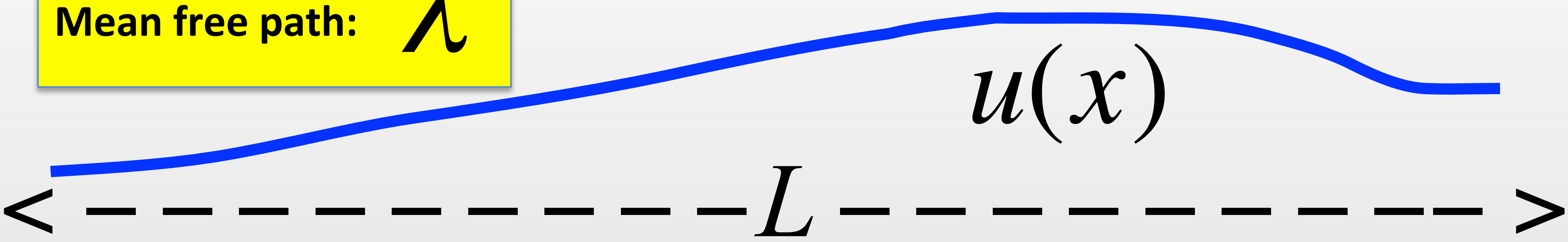


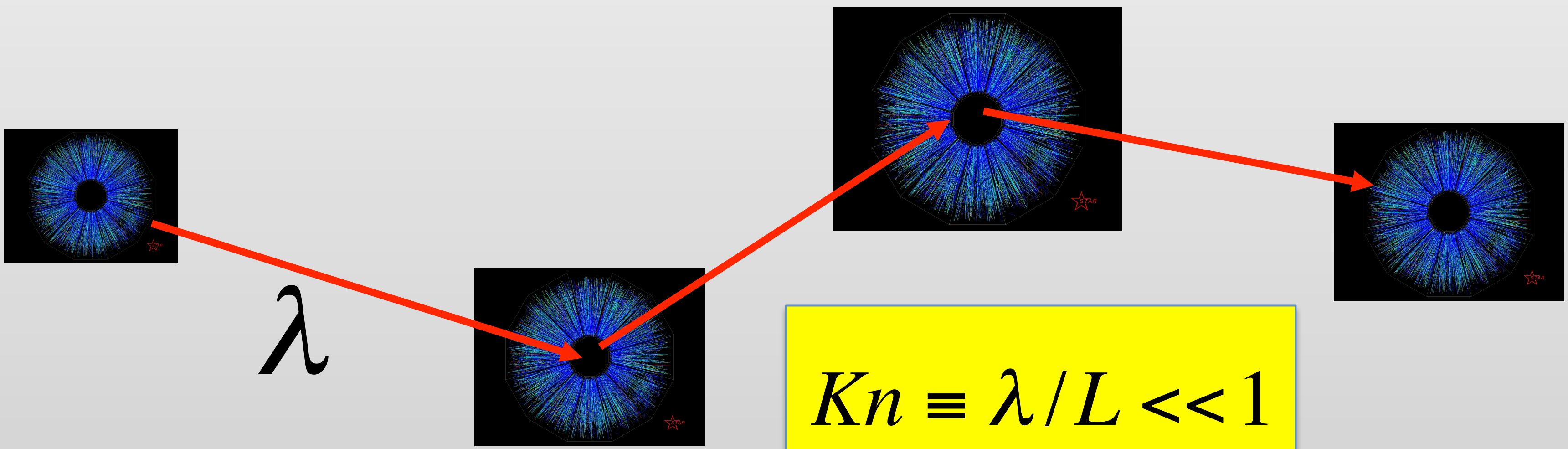
$$V_{th}^2 = kT/m$$

f^eq depends on space and time only through the macrofields: density **rho,** velocity **u** and temperature **T**: SLOW MODES

Non-equilibrium: the Knudsen number

Mean free path: λ





$$Kn \equiv \lambda / L << 1$$

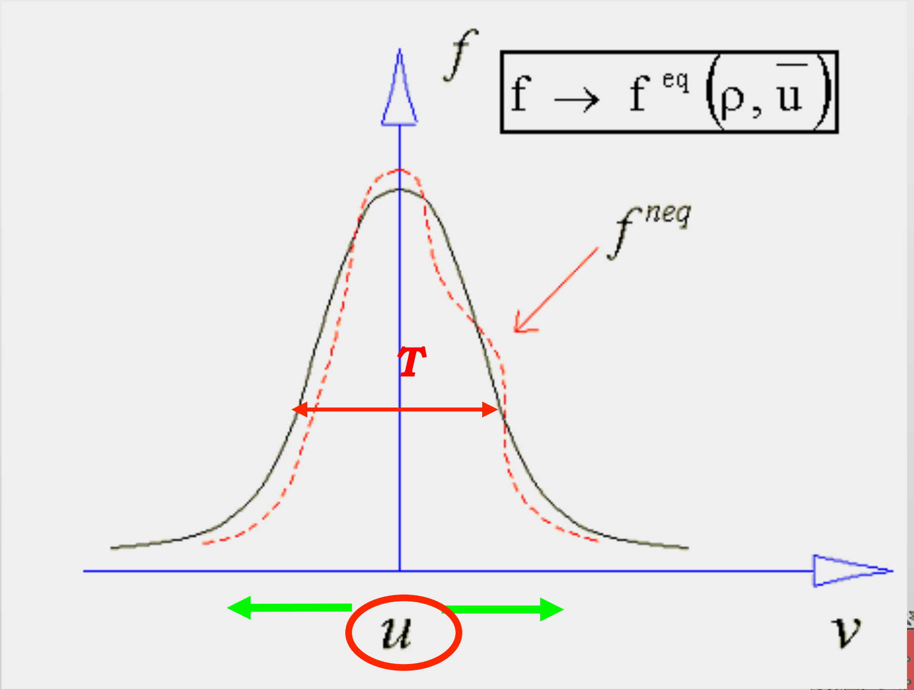
Any macrofield should change on scales much longer than the molecular one, i.e. mean free path, average length covered by a molecule between two subsequent collisions

Transport phenomena: weak non-equilibrium

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

Weak departure from local equilibrium (herd effect)

$$Kn = \left| \frac{f^{neq}}{f^{eq}} \right| << 1$$



Order params:

n=n(r,t)
u=u(r,t)
T=T(r,t)

- From kinetic theory to fluid dynamics,
- From Boltzmann to Navier-Stokes

Hydrodynamics: average over molecular velocities

$$\rho(\vec{r},t) = \int f(\vec{r},\vec{p},t)d\vec{p}$$

Mass density

$$J_a(\vec{r},t) = \int f(\vec{r},\vec{p},t)p_a d\vec{p}$$

Momentum density

$$P_{ab}(\vec{r},t) = \int f(\vec{r},\vec{p},t)p_a p_b d\vec{p}$$

Momentum Flux Tensor

$$Q_{abc}(\vec{r},t) = \int f(\vec{r},\vec{p},t)p_a p_b p_c d\vec{p}$$

Energy Flux Tensor

This is an endless hierarchy
Statistical closure required !

From Collisions to Relaxation

Close to equilibrium molecular details are "forgotten",

We can replace the true collision operator with a simple

Relaxation term

$$\boxed{Q = \frac{1}{\tau}(f^{eq} - f)}$$

The timescale **tau** controls the approach to equilibrium and dictates the transport coefficients (viscosity, thermal conductivity ….).

This is a good approx only close to local equilibrium, which is where Hydrodynamics lives …

From Boltzmann to Hydro I: Projection

1. Integrate the BE over increasing powers of p (tensors)

$$\int B[f]\,d\vec{p} \Rightarrow \qquad \partial_t \rho + \partial_a J_a = 0$$

$$\int B[f]\,p_a\,d\vec{p} \Rightarrow \qquad \partial_t J_a + \partial_b P_{ab} = 0$$

$$\int B[f]\,p_a p_b\,d\vec{p} \Rightarrow \qquad \partial_t P_{ab} + \partial_c Q_{abc} = \frac{1}{\tau}(P_{ab}^{eq} - P_{ab})$$

From Boltzmann to Hydro II: Weak Non-Equilibrium

2. Adiabatic/Weak non-equil closure

$$\partial_t P_{ab} + \partial_c Q_{abc} = \frac{1}{\tau}(P_{ab}^{eq} - P_{ab})$$

Within a timescale tau the momflux tensor relaxes to Equilibrium: the time derivative drops out and the energy flux tensor is also enslaved to equilibrium

$$\partial_c Q_{abc}^{eq} \approx \frac{1}{\tau}(P_{ab}^{eq} - P_{ab})$$

Inserting this in the equation for the current:

$$\underbrace{\partial_t J_a + \partial_b P_{ab}^{eq}}_{\text{(Advection)}} = \underbrace{\tau \partial_b \partial_c Q_{abc}^{eq}}_{\text{(Dissipation)}}$$

From Boltzmann to Hydro III: Local Equilibria

If feq is a local Maxwellian:

- $$P^{eq}_{ab} = \rho u_a u_b + p\delta_{ab}$$

  Advection+Equation of state:

- $$\tau \partial_c Q^{eq}_{abc} = 2\mu(\partial_a u_b + \partial_b u_a) + \lambda(\partial_c u_c)\delta_{ab}$$

  Mu and Lambda are known as shear and bulk viscosity.
  Note that this is a weak-gradient approx: nonequilibrium is proportional to the gradient of equilibrium.
  Linear Rheology (Newtonian Fluids)

Mission accomplished!

Applications

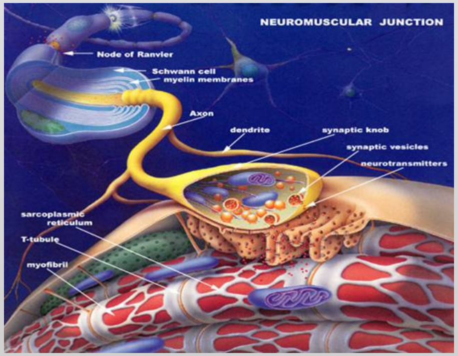
Systems far from local equilibrium

Neutron transport

Shock waves

Gamma rays transport

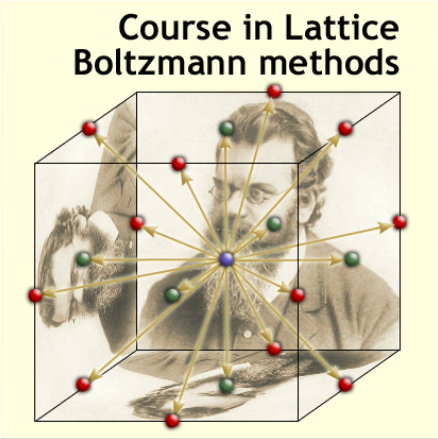
Shuttle re-entry



Electron flows

Traffic/cellular flows

From Boltzmann to Lattice Boltzmann



Boltzmann for fluids?
INSANE!!!

Why?

Lives in (6+1) dimensions !
Tough non-linear integro-differential equation

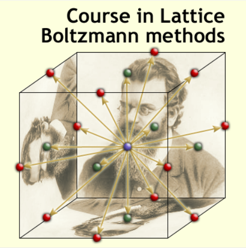
Computational suicide!

BUT …. it is definitely NOT, let's see why/how.

LB: fluids on phase-space-time crystals

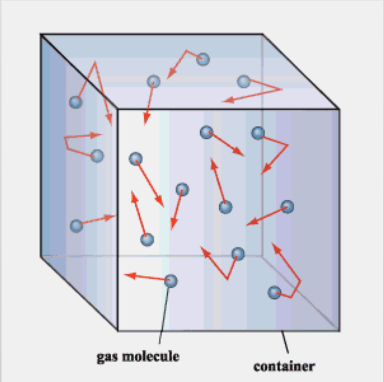
$m = 1$

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



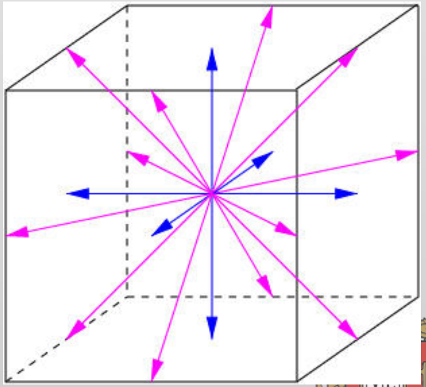
Momentum space is collapsed to a small set of discrete values

$$3d < b < 3^d$$



Universality

Individuality



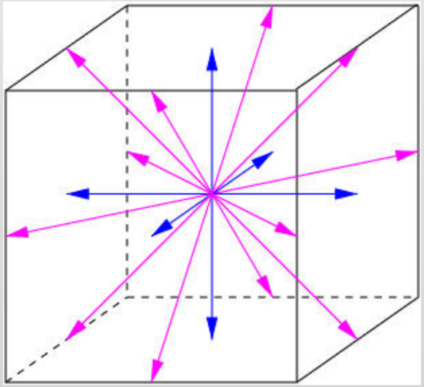
LB: fluids on phase-space-time crystals

$m = 1$

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

If the discrete momenta are chosen properly, hydro-fields are computed EXACTLY! It's Gauss quadrature…

$b = 18$



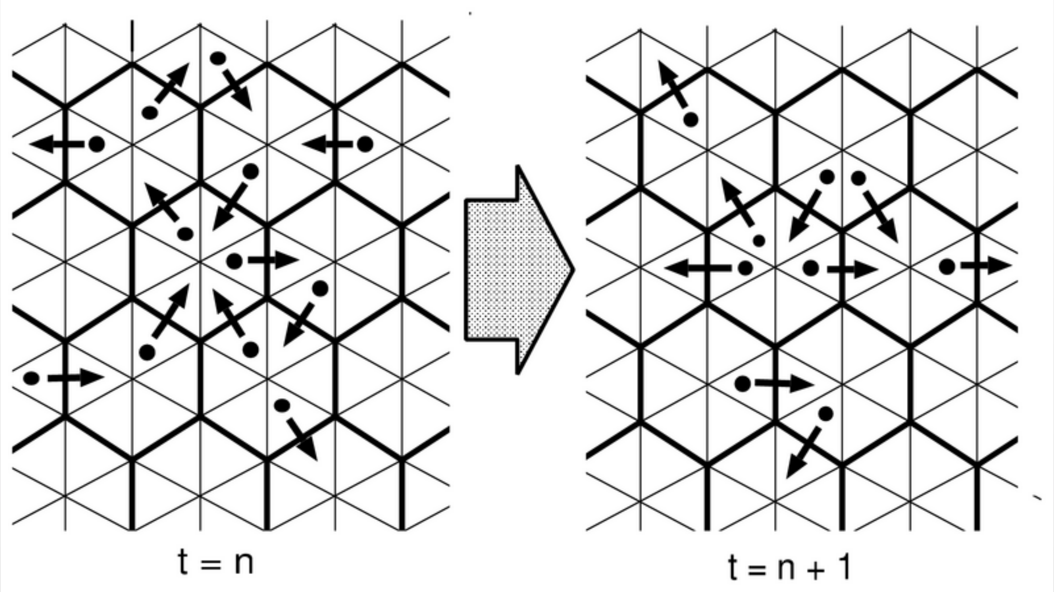
$$\rho(\vec{x};t) = \int f(\vec{x},\vec{p};t)\,d\vec{p} = \sum_{i=0}^{b} f_i(\vec{x};t)$$

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

The ancestor: Lattice Gas Cellular Automata

Boolean hydrodynamics!

$$n_i = \begin{cases} 0 & \text{absence} \\ 1 & \text{presence} \end{cases} \quad i = 0,6$$



$\Rightarrow$

$$\boxed{n_i\left(\vec{x} + \vec{c}_i, t + 1\right) - n_i\left(\vec{x}, t\right) = C_i(n)}$$

Frisch, Hasslacher, Pomeau, 1986, Wolfram, 1986

LB for 1d fluids

One-dimensional fluids: three macrofields: **rho,J,P**

$$\partial_t \rho + \partial_x J = 0 \qquad (J \equiv \rho u)$$

$$\partial_t J + \partial_x P = 0$$

Conservative: $$P^{con} = \rho u^2 + p(\rho)$$

Dissipative: $$P^{dis} \equiv \sigma = \rho \nu \partial_x u = \mu \partial_x u$$

1d fluids

By expressing **u*d/dt rho** using the continuity equation:

$$\partial_t \rho + u \partial_x \rho = -\rho \partial_x u$$

$$\rho(\partial_t u + u \partial_x u) = -\partial_x (p + \sigma)$$

Note that the density here is still alive, no **rho =const**. in d=1!

In the limit where pressure goes to zero (dust), we recover Burgers.

Density is still dynamic, and in d =1 it displays (non-linear) wavy features.
Metastable states (**d/dt rho ~ 0**), give **u=const./rho**, large velocity humps where rho is small and viceversa.
Since particles cannot overtake in d=1, this leads to strong compression/rarefaction regions.

LBE for 1d fluids

D1Q3 scheme: three velocities {-1,0,+1} in d=1

$$\{f_-, f_0, f_+\}$$

$$\left\{ \begin{array}{l} f_-(x - c\Delta t; t + \Delta t) - f_-(x;t) = -\Omega\Delta t[f_- - f_-^{eq}](x;t) \\ f_0(x; t + \Delta t) - f_0(x;t) = -\Omega\Delta t[f_0 - f_0^{eq}](x;t) \\ f_+(x + c\Delta t; t + \Delta t) - f_+(x;t) = -\Omega\Delta t[f_+ - f_+^{eq}](x;t) \end{array} \right.$$

"Particles" hop from site to site and collide (relax) around local equilibrium: **STREAM&RELAX** paradigm

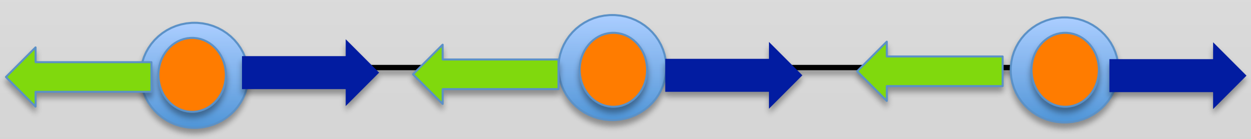
LB in compact form

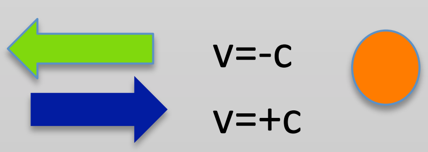
D1Q3: compact form

$$\boxed{f_i(x + c_i\Delta t; t + \Delta t) - f_i(x;t) = -\omega[f_i - f_i^{eq}](x;t)}$$

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

$c_1 = -1$ $\quad$ $c_2 = 0$ $\quad$ $c_3 = +1$





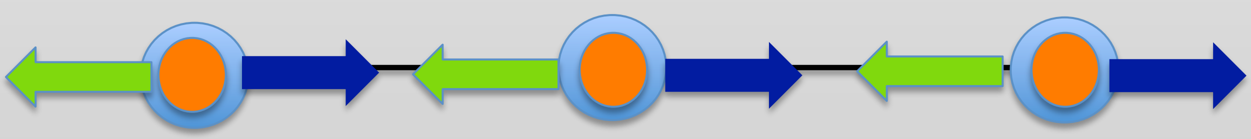
Semidiscrete LB

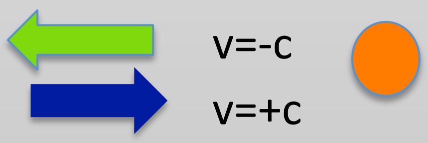
The macroscopic target is 1d hydrodynamics:

$$\partial_t(\rho u) + \partial_x(\rho u^2 + p) = \partial_x(\nu \partial_x(\rho u))$$

Taylor expand to 1° order in dt

$$\partial_t f_i + c_i \partial_x f_i = -\Omega[f_i - f_i^{eq}]$$





D1Q3: kinetic moments

A formal projection on {1,c,c^2} delivers a sequence of PDEs:

$$\sum_{i=-1,0,1} \cdots \qquad \partial_t \rho + \partial_x J = 0; \qquad \rho = \sum_{i=-1,0,1} f_i \quad J = \sum_{i=-1,0,1} f_i c_i$$

$$\sum_{i=-1,0,1} c_i \cdots \qquad \partial_t J + \partial_x P = 0; \qquad P = \sum_{i=-1,0,1} f_i c_i^2$$

$$\sum_{i=-1,0,1} c_i^2 \cdots \qquad \partial_t P + \partial_x Q = -\Omega(P - P^{eq}); \qquad Q = \sum_{i=-1,0,1} f_i c_i^3$$

D1Q3: enslaving

$$\partial_t \rho + \partial_x J = 0$$

Target: Hydrodynamic eqs in d=1

$$\boxed{\partial_t(\rho u) + \partial_x(\rho u^2 + p) = \partial_x(\nu \partial_x(\rho u))}$$

$$\partial_t J + \partial_x P = 0$$

Enslaving + P close to equilibrium

$$P \approx P^{eq} - \tau \partial_x Q \approx P^{eq} - \tau \partial_x Q^{eq} \qquad (\tau \equiv 1/\Omega)$$

Insert this back into the equation for the current:

$$\partial_t J + \partial_x P^{eq} = \tau \partial_x^2 Q^{eq}$$

LB viscosity

By comparing with NSE, we recover d=1 hydrodynamics iff:

$$(\nu = c_s^2 \tau)$$

$$\boxed{P^{eq} = \rho u^2 + p \qquad \tau Q^{eq} = \rho \nu u}$$

D1Q3: local equilibria

Mass-Momentum Conservation:

$$\{f_-, f_0, f_+\}$$

3 fields require (at least) 3 movers

$$\begin{cases} f_-^{eq} + f_0^{eq} + f_+^{eq} = \rho \\ c(-f_-^{eq} + f_+^{eq}) = J = \rho u \\ c^2(f_-^{eq} + f_+^{eq}) = P^{eq} = p + \rho u^2 \neq P \end{cases}$$

Momentum-Flux is **Not** Conserved!

Multiply (2)*c and sum (3):

$$\begin{cases} f_-^{eq} = (p - Jc + Ju)/2c^2 \\ f_+^{eq} = (p + Ju + Jc)/2c^2 \\ f_0^{eq} = (\rho c^2 - pc - Ju^2)/c^2 \end{cases}$$

Fluid dynamics

The 3x3 system delivers the local equilibria:

$$
\begin{cases}
f_{+}^{eq} = \rho(W^2 - \beta + \beta^2)/2 \\
f_{+}^{eq} = \rho(W^2 + \beta + \beta^2)/2 \\
f_{0}^{eq} = \rho(1 - W^2 - \beta^2)
\end{cases}
$$

Equation of State:

$$\boxed{p = \rho c_s^2}$$

Where:

$$\boxed{\begin{aligned} W &\equiv c_s / c \\ \beta &\equiv u / c \end{aligned}}$$

Equation of state, sound/light speed: free parameter ("Temperature")

"Relativistic fluid/light speed"

The relativistic flavor is unsurprising because particles move at the light speed **c=dx/dt**: (Weyl fermions)!

“Thermodynamic” EoS

Mass-momentum at **zero flow (u=0)** $W = c_s / c$

$$f_{-}^{eq} = \frac{\rho W^2}{2} \qquad f_{+}^{eq} = \frac{\rho W^2}{2} \qquad f_{0}^{eq} = \rho(1 - W^2)$$

This naturally defines a set of weights:

$$\{w_-, w_0, w_+\} = \{\frac{W^2}{2}, (1 - W^2), \frac{W^2}{2}\}$$

They are the lattice **analogues** of canonical Boltzmann weights

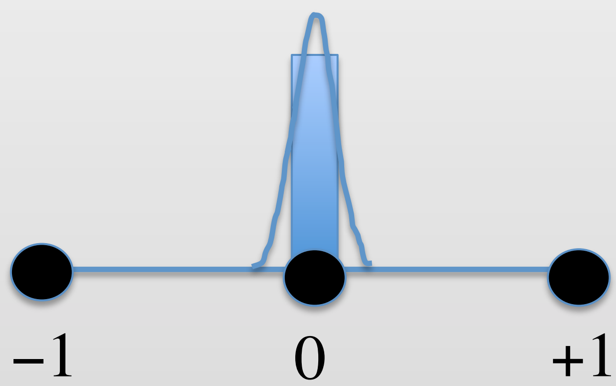
$$w(E) = e^{-E/k_b T}$$

These are just “analogues” because there is no continuum distribution in velocity space. **No standard thermodynamics!**

Equils: athermal fluid

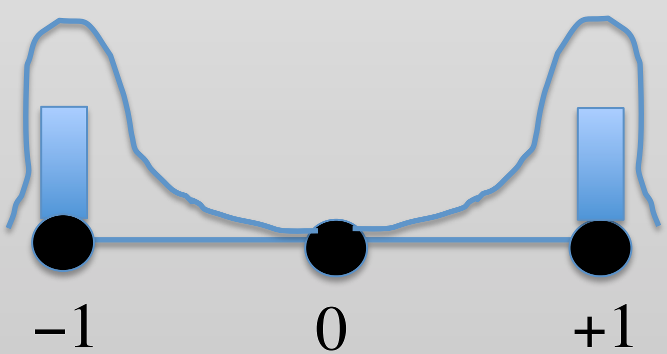
$$\{w_-, w_0, w_+\} = \{\frac{W^2}{2}, (1 - W^2), \frac{W^2}{2}\}$$

$W = 0$



T=0 “ Bose Condensation”

$W = 1$

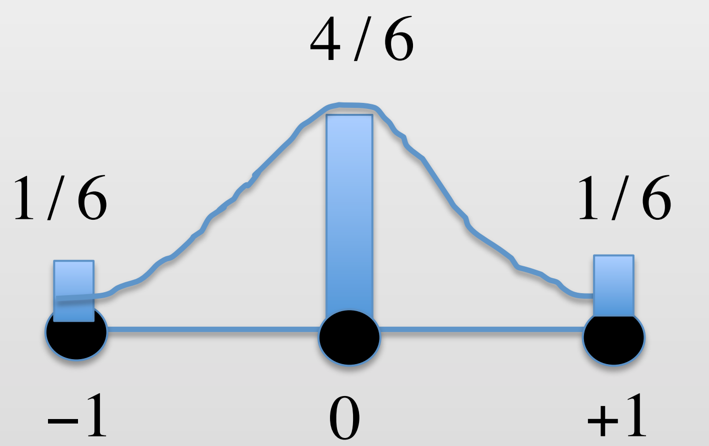


T=1 “Quark-gluon plasma”

Equils: athermal fluid

$$\{w_{-1}, w_0, w_+\} = \{\frac{W^2}{2}, (1 - W^2), \frac{W^2}{2}\}$$

$W^2 = 1/3$



T=1/3 “Maxwell-Boltzmann”

This is the LB equation of State= Relativistic Radiation!

$$\boxed{\frac{c_s^2}{c^2} = W^2 = 1/3}$$

Transport: Dissipation

The dissipative constraint to recover Navier-Stokes is:

$$\tau Q^{eq} = \rho \nu u$$

Namely:

$$\tau \sum_{i=-1}^{+1} c_i^3 f_i^{eq} = \rho \nu u$$

Namely:

$$\tau c^3 (-f_-^{eq} + f_+^{eq}) = \tau c^3 \frac{\rho W^2}{2} (u + u) / c$$

$$\tau Q^{eq} = \tau c^2 \rho W^2 u \equiv \rho u \nu$$

$$\boxed{\nu = c^2 W^2 \tau = c_s^2 \tau}$$

q.e.d.

LBE: Upsides

What did we gain?

First order in space and time

Equilibria are local: round-off precision, no space-derivatives!

Pressure and Stress are local:

Streaming is along lightcones, not the material lines: EXACT

Negative numerical diffusion (higher order terms)

Small dispersion (c*dt=dx)

Complex geometries (visible in d>1)

Parallel computing (visible in d>1)

LBE: downsides

What did we loose?

Holds only under enslaving and weak departure from local equilibrium

More memory

Uniform lattices

Fixed time-step

The upsides become much more compelling in d>1: next lecture!

Assignments

1. **Write a d1q3 LB code for 1d fluids**
   and comment the dynamics as a function of omega
   Hint: choose omega well within 0 < omega < 2.

2. **Do the same with different Quark-Gluon plasma and**
   Bose-Einstein weights: do you ever loose stability?
   Hint: the actual LB viscosity is nu=cs^2*(tau-dt/2)

End of the lecture