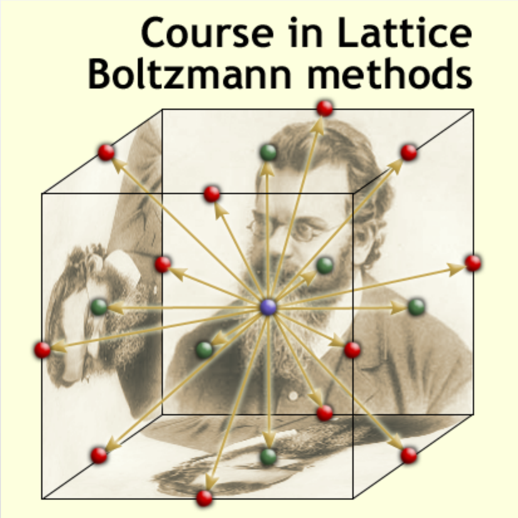
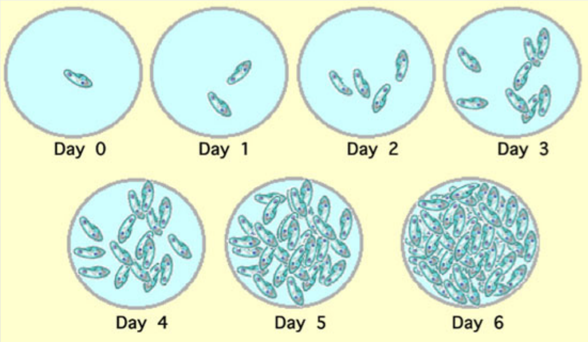
Lattice Boltzmann for ADR

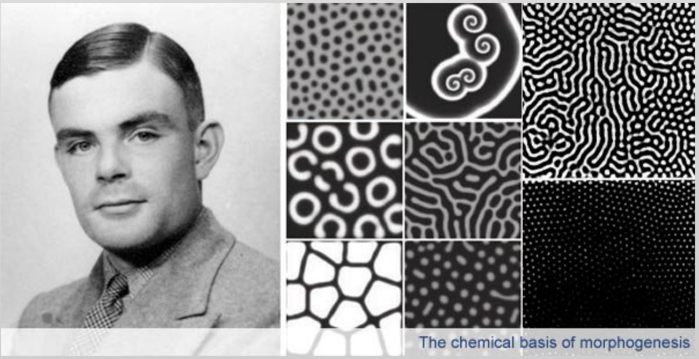


Sauro Succi

Advection-Diffusion-Reaction

A lot of KEY applications in science and engineering (combustion, crystal growth, population bacteria dynamics...





LB for 1d ADR

One-dimensional Advection-Diffusion-Reaction

$$\boxed{\partial_t \rho + U \partial_x \rho = D \partial_{xx} \rho + R(\rho)}$$

Conservative Form:

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

Conservative: $$J^{con} = \rho U$$

Dissipative: $$J^{dis} = -D \partial_x \rho$$

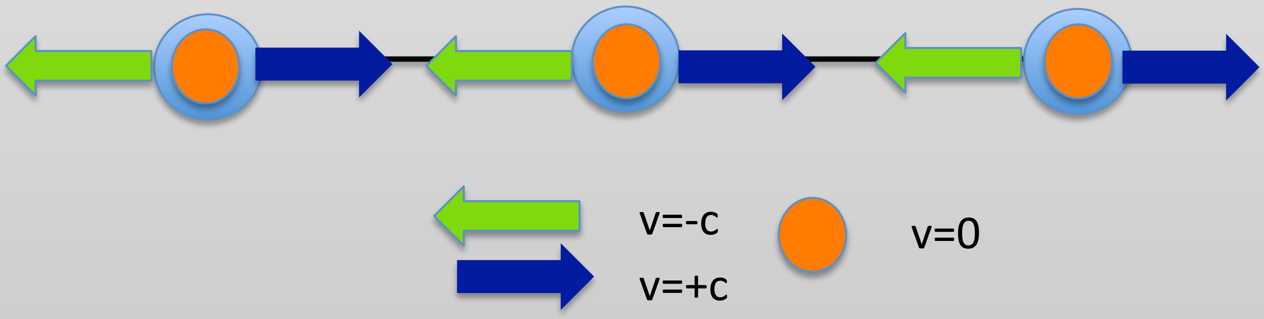
Source: $$S = R(\rho)$$

Semidiscrete LB

$$f_i(x + c_i dt; t + dt) - f_i(x,t) = -\Omega[f_i - f_i^{eq}]dt + R_i dt$$

Taylor expand to 1° order in dt

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



D1Q3: kinetic moments

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

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

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

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

D1Q3: enslaving

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

$$\partial_t J + \partial_x P = -\omega (J - J^{eq})$$

Momentum is NOT conserved

Enslaving J close to equilibrium

$$J \sim J^{eq} - \tau \partial_x P^{eq}$$

$$(\tau \equiv 1/\Omega)$$

Insert this back into the equation for the current:

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

LB viscosity

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

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

$$J^{eq} = \rho U \qquad P^{eq} = \rho c_s^2$$

D1Q3: local equilibria

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

Mass Conservation:

2 fields require (at least) 2 movers

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

Current is **Not** Conserved!

Momentum-Flux is **Not** Conserved!

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

$$\begin{cases} f_-^{eq} = \rho(-U/c + c_s^2/c^2)/2 \\ f_+^{eq} = \rho(+U/c + c_s^2/c^2)/2 \\ f_0^{eq} = \rho(1 - c_s^2/c^2) \end{cases}$$

Fluid dynamics

The 3x3 system delivers the local equilibria:

$$\begin{cases} f_-^{eq} = \rho(W^2 - \beta)/2 \\ f_+^{eq} = \rho(W^2 + \beta)/2 \\ f_0^{eq} = \rho(1 - W^2) \end{cases}$$

Diffusivity:

$$\boxed{D = c_s^2 \tau}$$

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

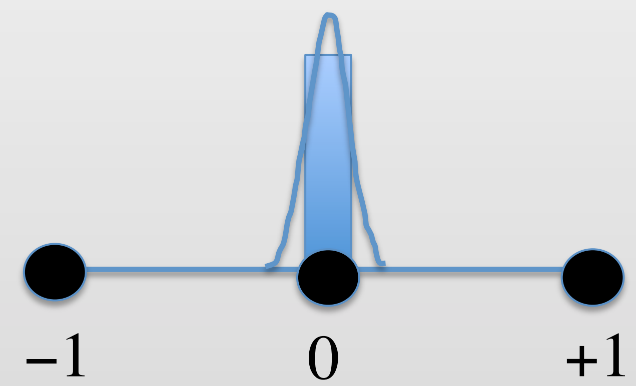
$$w(E) = e^{-E/k_b T}$$

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

Chemical Reaction

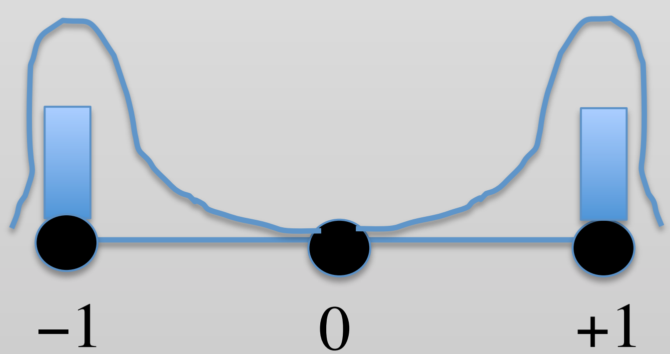
$$\{R_-, R_0, R_+\} = \{\frac{W^2}{2}, (1-W^2), \frac{W^2}{2}\} R(\rho)$$

$W = 0$



T=0 " Bose Condensation"

$W = 1$

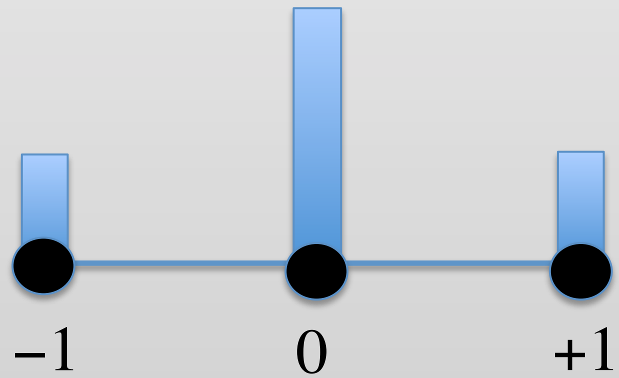


T=1 "Quark-gluon plasma"

Equils: athermal fluid

$$\{R_-, R_0, R_+\} = \{\frac{W^2}{2}, (1 - W^2), \frac{W^2}{2}\} R(\rho)$$

As simple as that!

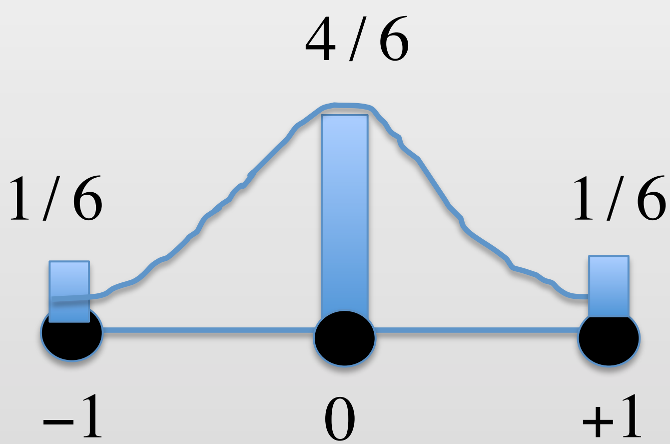


The rest population permits to adjust the sound speed. With only left and right movers cs=c

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!

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

Assignments

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

2. **Write a D1Q3 code for the ADR with logistic reactions**
   R = a*rho-b*rho^2
   and comment the solutions

3. Make **a** random with negative average but
   positive fluctuations > **b.**
   Comment the solutions

End of the lecture