diffusion

v $v+dv$

random changes $\propto \rho(x,v)$

flux $\propto \rho(v+dv) - \rho(v) \quad \propto \frac{\partial \rho}{\partial v}$

$d\rho\, dv \propto dt \left[\frac{\partial\rho}{\partial v}(v+dv) - \frac{\partial\rho}{\partial v}(v)\right]$

v $v+dv$

stationary solution

$$\rho \propto \exp(-\beta(V(x) + \tfrac{1}{2}mv^2)) \quad \text{(Boltzmann factor)}$$

$$\frac{d}{dt}\rho(x,v) = 0 = (a(x) - \eta v)(-\beta m v)\rho - \eta\rho + v(-\beta V')\rho$$
$$+ \frac{\partial}{\partial v}(-\beta m v)\rho D_{vv}$$

$$[\cancel{a(x)} - \eta v](-\beta m v)\rho - \eta\rho + -\beta m\rho D + (-\beta m v)^2 \rho D$$

$$= \rho(\eta\beta m v^2 - \eta - \beta m D + \beta^2 m^2 v^2 D)$$

$$= 0 \quad \text{if} \quad \eta = D\beta m$$

$\Rightarrow$ correct ensemble averages enforced.

Nosé-Hoover   Deterministic   Very common

additional variable s for heat bath

some parameter

$$H_{Nos\acute{e}} = \mathcal{H}' + \frac{p_s^2}{2Q} + L\frac{\log s}{\beta}$$

$$\mathcal{H}' = \frac{p_i^2}{2m_i s^2} + U(r_1 \dots r_N)$$

$p' = p/s$

$\mu(\gamma)$ is micro cannonical, constant E, N, V

$\delta[H_{Nose} - E]$ .... algebra ... integrating out s

$$\Rightarrow \langle A(p/s, r)\rangle_{Nose} = \langle A(p', r)\rangle_{NVT} \quad \text{canonical!}$$

Hoover rewrote it intelligently to make it easier to implement

Not Hamiltonian

$$\dot{r}_i = p_i/m \qquad \dot{p}_i = a(r_1 \dots r_N) - \xi p_i$$

effective friction

$$\dot{\xi} = \left(\sum p_i^2/m_i - \frac{L}{\beta}\right)/Q$$

$\leftarrow$ difference to temp you want.

$$\frac{\dot{s}}{s} = \frac{d}{dt}\log s = \xi$$

$\leftarrow$ redundant, but nice for checking ($H_{Nosé}$ conserved)

Notes: - log(s) was necessary to get correct behaviour

- necessary to have only one constant of motion, otherwise Nosé-Hoover chains. (due to δ function)

$\longleftrightarrow$ thermostat coupled to more thermostats

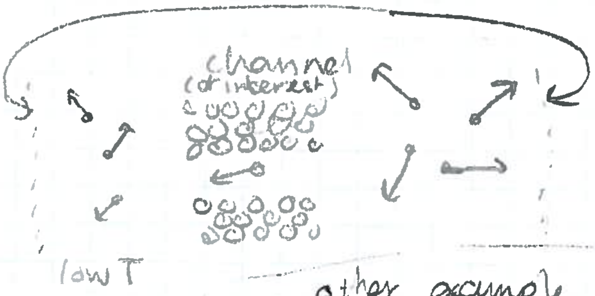
- global dependance.

Applying thermostats

- choose carefully. What is more realistic?
- where to apply? Far away from relevant dynamics.
- careful with out-of-equilibrium systems
  $g(r)$ is not the only thing that needs to be ok.
- There are other options (i.e to damp phonons)

example

periodic

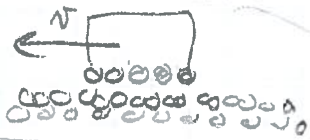


How would you thermostat this?

Will get exercises on thermostats!

How would you thermostat LJ Argon liquid?

other example



Barostats etc

scheme similar to Nosé-Hoover: include volume as variable. read the book section 6.2

In general: key to something-o-stat is
to produce correct $g(r)$

Monte-Carlo (with randomness)

- direct MC: replace some physics by random process
- MC integration: use to calculate integrals
- "metropolis" MC: Markov chains

(slightly blurry boundaries).

Direct MC: usually ad-hoc-ish

f.e random Lorentz gas
draw random collision params for next scatterer

f.e Langevin thermostat: heat bath → random noise + damping

end lecture 7

f.e simple traffic model: Nagel - Schreckenberg

$v=3$ $v=4$ $v=$

road is 1d grid with cars + vel.
some max saf velocity v_{max}

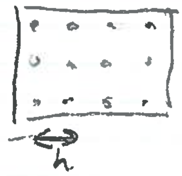
1) cars accelerate by 1: $v_i{+}{+}$
2) if distance to car in front $(x_{i+1}-x_i) < v_i$: $v_i = x_{i+1}-x_i-1$
3) $v \leq v_{max}$
4) with probability p $v_i{-}{-}$ ← driver choice, or sillyness or whatever
5) if $v_i < 0$: $v_i = 0$

⇒ widely studied, + additions, explains a lot of qualitative behaviour of traffic jams. real traffic $v_{max} \approx 5$

MC integration

$\int dx\, f(x)$ ← smooth

hopefully from num. methods course



- usual integration methods based on regular grid
  to improve: points closer together (decrease h)
  (methods using interpolation described in Thyssen's appendix) $O(h^k)$ for some k.
- MC: instead of grid, random points
  after N points error $= O\left(\frac{1}{\sqrt{N}}\right)$

$\int dx\, f(x) \approx \text{area}\, \langle f(x) \rangle \approx \frac{\text{area}}{N} \sum_{i=1}^{N} f(x_i)$

in d dimension

grid	MC
$N \propto \left(\frac{1}{h}\right)^d$ ← high dimensional ⇒ many points	
error $O\left(\frac{1}{N}\right)^{k/d}$	$O\left(\left(\frac{1}{N}\right)^{1/2}\right)$

⇒ if $k/d < 1/2$ MC is better