Finite thermostats in nonequilibrium Statistical Mechanics

Progress due to

(a) Study of stationary states out of equilibrium (as opposed to deviation and return to equilibrium), [EM89].
(b) Modeling thermostats in terms of finite systems, [DGM84],[No84],[Ho85]

Finite thermostats have been essential. Rationale: the properties of the system should not depend on the special way thermostats are imagined to work.

Equations of motion are NOT Hamiltonian.

Mechanical interpretation of phase space contraction:

$$\sigma(x) \stackrel{def}{=} -\operatorname{div} f(x) = -\sum_{j=1}^{3N} \partial_i f_i(x)$$

"Empirical fact": $\sigma(x)$ is related to the *phase space contraction*. Not equal because $\sigma(x)$ is not intrinsic: changing metric

$$\sigma'(x) = \sigma(x) - \frac{d}{dt}\Gamma(x)$$

so that only time averages over long times can have "intrinsic" meaning:

$$\frac{1}{\tau}\int_0^\tau \sigma'(S_t x)dt = \frac{1}{\tau}\int_0^\tau \sigma(S_t x)dt + \frac{\Gamma(S_\tau x) - \Gamma(x)}{\tau} \xrightarrow[\tau\to+\infty]{} \frac{1}{\tau}\int_0^\tau \sigma(S_t x)dt$$

The average

$$\sigma_+ \stackrel{def}{=} \lim_{\tau\to+\infty} \frac{1}{\tau}\int_0^\tau \sigma(S_t x)dt$$

has been identified with entropy creation rate

$$\sigma_+ = \langle \sum_j \frac{Q_j}{T_j} \rangle$$

Several reasons: for instance consider the thermostat model

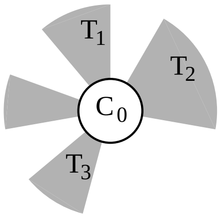


fig.1

Fig.1: Particles in $\mathcal{C}_0$ ("system particle") interactwith the particles in the shaded regions ("thermostats particles") which are constrained to have a fixed total kinetic energy.

The equations of motion will be (all masses equal for simplicity)

$$\begin{aligned} m\ddot{\mathbf{X}}_0 =& -\partial_{\mathbf{X}_0}\Big(U_0(\mathbf{X}_0)+\sum_{j>0} W_{0,j}(\mathbf{X}_0,\mathbf{X}_j)\Big)+\mathbf{E}(\mathbf{X}_0),\\ m\ddot{\mathbf{X}}_i =& -\partial_{\mathbf{X}_i}\Big(U_i(\mathbf{X}_i)+W_{0,i}(\mathbf{X}_0,\mathbf{X}_i)\Big)-\alpha_i\dot{\mathbf{X}}_i \end{aligned}$$

with α_i such that K_i is a constant. Here $W_{0,i}$ is the interaction potential between particles in $\mathcal{C}_i$ and in $\mathcal{C}_0$, while U_0, U_i are the internal energies of the particles in $\mathcal{C}_0, \mathcal{C}_i$ respectively. We imagine that the energies $W_{0,j}, U_j$ are due to *smooth* translation invariant pair potentials; repulsion from the boundaries of the containers will be elastic reflection. It is assumed that there is no direct interaction between different thermostats: their particles interact directly only with the ones in $\mathcal{C}_0$. Here $\mathbf{E}(\mathbf{X}_0)$ denotes possibly present external positional forces stirring the particles in $\mathcal{C}_0$. The contraints on the thermostats kinetic energies give

$$\alpha_i \equiv \frac{Q_i - \dot U_i}{3N_i k_B T_i} \qquad \longleftrightarrow \qquad K_i \equiv const \stackrel{def}{=} \frac{3}{2} N_i k_B T_i$$

where the work per unit time that particles outside the thermostat $\mathcal{C}_i$ (hence in $\mathcal{C}_0$) exercise on the particles in it, is

$$Q_i \stackrel{def}{=} -\dot{\mathbf{X}}_i \cdot \partial_{\mathbf{X}_i} W_{0,i}(\mathbf{X}_0, \mathbf{X}_i)$$

The model identifies the "temperature of the thermostats" with their total kinetic energy via $K_i \stackrel{def}{=} \frac{3}{2} N_i k_B T_i$ which is possible since K_i is a constant of motion.
Hence

$$\sigma(\mathbf{X}, \dot{\mathbf{X}}) \equiv \varepsilon(\mathbf{X}, \dot{\mathbf{X}}) + \dot R(\mathbf{X}, \dot{\mathbf{X}})$$

and

$$\varepsilon(\mathbf{X}, \dot{\mathbf{X}}) = \sum_{j=1}^{n} \frac{Q_j}{k_B T_j}$$

Measurable by calorimetric and thermometric experiments: independent of the equations of motion.

Useful? Fluctuations in average

$$\frac{1}{T}\int_0^T \sigma(S_t x) \equiv \frac{1}{T}\int_0^T \varepsilon(S_t x) + \frac{R(T) - R(0)}{T}$$

Therefore for large T *same flactuations statistics.*

$$\langle \sigma \rangle \equiv \langle \varepsilon \rangle$$

A general theory of fluctuations of $\sigma \longleftrightarrow$ general theory of fluctuations of ε

Chaotic hypothesis (CH): *Motions developing on the attracting set of a chaotic system can be regarded as motions of a transitive hyperbolic (also called "Anosov") system.*

(1) Existence of time averages and their statistics μ (SRB statistics)

$$\frac{1}{T}\int_0^T F(S_t x)\,dt \xrightarrow[T\to\infty]{} \int_{\mathcal{A}} F(y)\mu(dy) \stackrel{def}{=} \langle F\rangle$$

(2) Coarse graining is rigorously definable and SRB is, consequently, interpretable as equidistribution on the attracting set ($\Rightarrow$ variational principle and existence of Lyapunov function)
(3) μ admits an explicit representation so that averages can be written and compared (without computing them)
(4) large deviations law holds: $f_j \stackrel{def}{=} \frac{1}{\tau}\int_0^\tau F_j(S_t x)dt$

$$Prob(\mathbf{f}\in\Delta) = Prob((f_1,\ldots,f_n)\in\Delta) \propto_{\tau\to\infty} e^{\tau\max_{\mathbf{f}\in\Delta}\zeta(\mathbf{f})}$$

ζ defined in a convex open set Γ and analytic there and $\zeta = -\infty$ outside $\overline{\Gamma}$

(6) in *time reversal invariant* cases FT: (F_j odd)

$$\zeta(-\mathbf{f}) = \zeta(\mathbf{f}) - \langle\varepsilon\rangle \qquad \longleftrightarrow \qquad \frac{Prob(\mathbf{f})}{Prob(-\mathbf{f})} = e^{p\sigma_+\tau}$$

provided $\sigma = \varphi(\mathbf{F})$ and $\langle\varepsilon\rangle > 0$ (e.g. $F_1 = \sigma$. No free parameters. More surprisingly

$$\frac{Prob_\mu(F_j(S_t x)\sim\varphi(t),\,t\in[0,\tau])}{Prob_\mu(F_j(S_t x)\sim-\varphi(\tau-t),\,t\in[0,\tau])} \propto e^{\int_0^t \sigma(S_t x)dt}$$

Applications (to fluids)
(1) Fluid equations are not reversible. Equivalence conjecture:

$$\dot{\mathbf{u}} + \underset{\sim}{\mathbf{u}} \cdot \underset{\sim}{\partial}\, \mathbf{u} = \nu \Delta \mathbf{u} - \partial\, p + \mathbf{g},$$

$$\dot{\mathbf{u}} + \underset{\sim}{\mathbf{u}} \cdot \underset{\sim}{\partial}\, \mathbf{u} = \alpha(\mathbf{u}) \Delta \mathbf{u} - \partial\, p + \mathbf{g}, \qquad \alpha = \frac{\int \mathbf{u}\cdot\mathbf{g}}{\int (\partial\, \mathbf{u})^2} \;\Rightarrow\; \int \mathbf{u}^2 = \mathcal{E} = const$$

Same statistics for "local observables": F local $\Rightarrow$ F depends on finitely many Fourier comp. of $\mathbf{u}$.

Same statistics $\Rightarrow$ as $R \to \infty$ if $\mathcal{E}$ is chosen $= \langle \int \mathbf{u}^2 \rangle_{\mu_\nu}$ (equivalence): "Gaussian NS eq." or "GNS". So far *only numerical tests in strongly cut off equations and* $d = 2$ (Rondoni,Segre).

Problem: can reversibility be detected?
Assume K41
then the number of degrees of freedom is the momenta with $|\mathbf{k}| < R^{\frac{3}{7}4}$
Divergence $\sigma \sim \nu \sum_{\mathbf{k}} 2|\mathbf{k}|^2 = \nu\, (\frac{2\pi}{L})^2 \frac{8\pi}{5} R^{15/4}$
By FT probability (relative) to see wrong friction for a time τ is

$$P \sim e^{-\tau\nu \frac{32\pi^3}{L^2} R^{\frac{1}{5}4}}$$

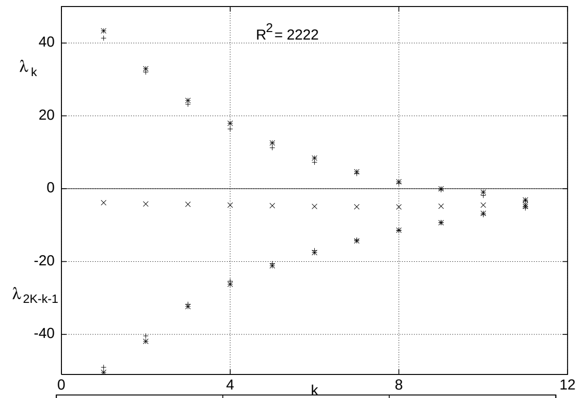
So (air)

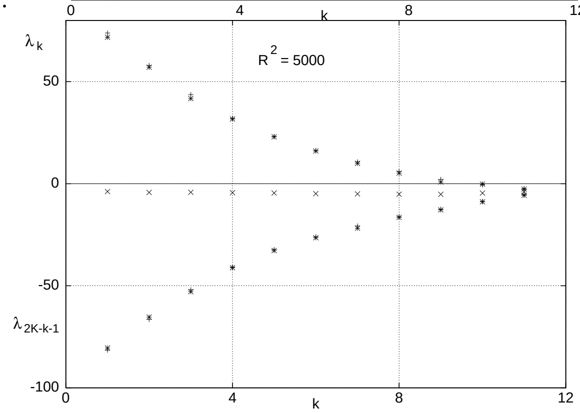
$$\begin{aligned} &\text{CGS units (data for air)}\\ \nu =& 1.5\, 10^{-2}, \quad v = 10. \quad L = 100.\\ R =& 6.67\, 10^4, \quad g = 3.66\, 10^{14}\\ P =& e^{-g\tau} = e^{-3.66\, 10^8}, \qquad \text{if} \quad \tau = 10^{-6} \end{aligned}$$

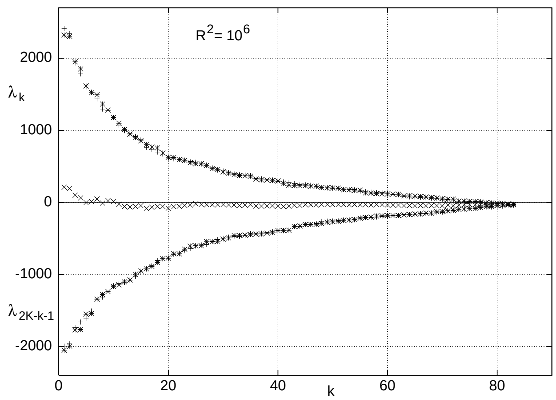
Viscosity is $-\nu$ during $10^{-6}s$ with probability $e^{-.25\, 10^6}$: similar to the recurence times calculatioon

Compatibility? near equil. entropy creation independently defined (DeGroot-Mazur)

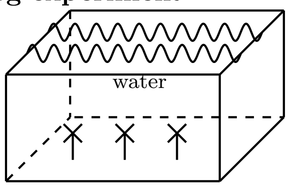
$$k_B\langle\varepsilon\rangle = k_B\varepsilon_{classic}+\dot{S},\qquad k_B\varepsilon_{classic}=\int_{\mathcal{C}_0}\Big(\kappa\,\big(\frac{\partial T}{T}\big)^2+\eta\,\frac{1}{T}\underset{\sim}{\boldsymbol{\tau}}'\cdot\underset{\sim}{\partial}\mathbf{u}\Big)\,d\mathbf{x}$$







Bandi-Cressman-Goldburg experiment



Lagrangian flow *on a 2D surface*
$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t)$
with $\mathbf{u}$ turbulent
"Kraichnan flow (space-time colored)"

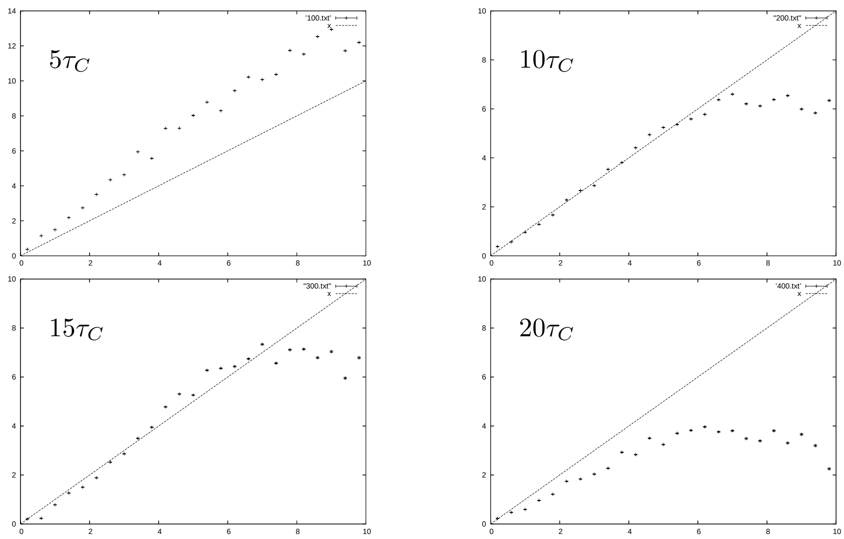
Turbulent water in $1m \times 1m \times 0.3m$. Generate "Lagrangian trajectories" on surface

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t)$$

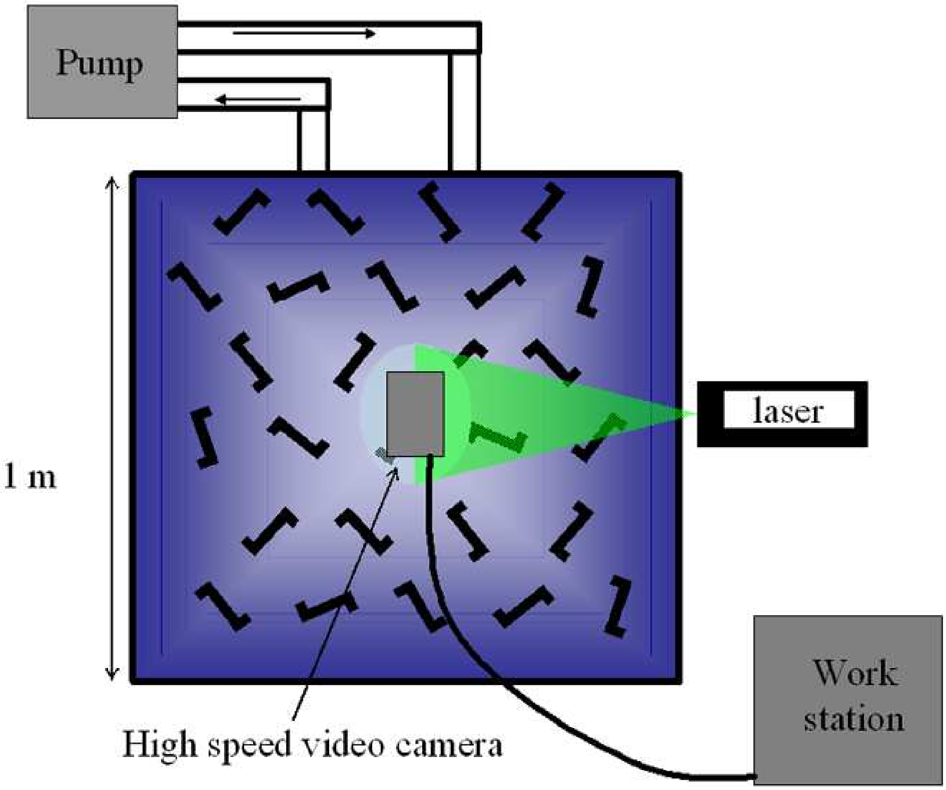
$\sigma(\mathbf{x}(t), t) = -\mathrm{div}\mathbf{u}(\mathbf{x}(t), t)$ whose time av. is exper. measured to be $\sigma_+ = \Omega > 0$.

$$p = \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{x}(t), t)}{\Omega}\, dt, \qquad ? \qquad \zeta(-p) = \zeta(p) - p\,\Omega$$

for $\tau \gg \tau_c =$ "characteristic time of turbulence evolution".
(1) a definitely non Gaussian statistics for the variable $p = \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{x}(t),t)}{\Omega} dt$.
(2) remarkably large fluctuations of p for values of τ up to $800ms$.
(3) the obstacle of not knowing the quantity p because the equations of motion are usually not known is not present: FR prediction, no free parameters.
(4) the statistics is quite large as about 8×10^4 Lagrangian trajectory staying in the field of vision for a time length $T = 6$s are observed. Dividing T into $k = T/\tau$ "segments", with time duration τ, $8 \times 10^4\, k$ averages of velocity divergences are obtained, with k varying between 60 and 15 (where 60 corresponds to $\tau = 100$ms). Small statistics so far had been a major obstacle to FR tests.
Theory: Chetrite,Delannoy,Gawedzki, Bonetto,Gentile,G.



$5\tau_C$
'100.txt'
x
$10\tau_C$
"200.txt"
x
$15\tau_C$
"300.txt"
x
$20\tau_C$
'400.txt'
x


Pump
laser
1 m
Work
station
High speed video camera