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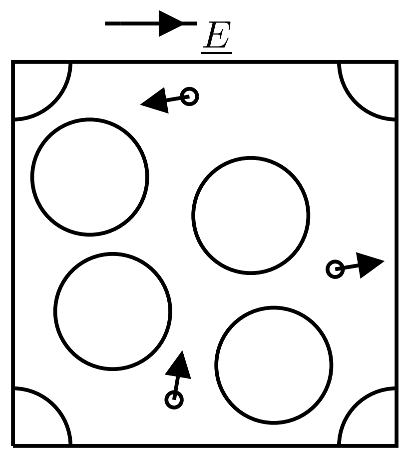
Nonequilibrium Stationary States

System subject to nonconservative forces: hence to thermostats. Example



$\underline{E}$ external non conservative force

$$m\,\ddot{\underline{x}}_i = \underline{F}_i + \underline{E} - \underline{\vartheta}_i$$

$\underline{\vartheta}$ thermostat force

$\underline{\vartheta}$ thermostat models

(1) $\underline{\vartheta}_i = -\nu\,\underline{p}_i$ (viscous thermostat)

(2) $\underline{\vartheta}_i = -\alpha\,\underline{p}_i \qquad \alpha = \frac{\sum \dot{\underline{x}}_i\cdot \underline{E}}{\sum \underline{p}_i^2/m}$ (Gaussian thermostat)

(3) anelastic $\sqrt{\eta}$ = restitution coefficient ($\underline{v}\cdot\underline{n} \to -\sqrt{\eta}\,\underline{v}\cdot\underline{n}$

(4) renormalize $|\underline{v}_i|$ after each collision to $|\underline{v}'_i| = \sqrt{\frac{d}{2}\frac{k_BT}{m}}$

(5) stochastic thermostat and infinite reservoir thermostat (Rey Bellet)

Thermostats $\longleftrightarrow$ phase space contraction $\sigma = -\mathrm{div}\,\underline{\vartheta} = -\sum \partial_{\underline{p}_i}\underline{\vartheta}_i(x,p)$

(1) $\sigma = \nu\,N\,d$

(2) $\sigma = N\frac{\sum \underline{E}\cdot\dot{\underline{x}}_i}{k_BT} = N\frac{L}{k_BT_\vartheta}$ if $N\frac{d}{2}k_BT \stackrel{def}{=} \sum \frac{\underline{p}_i^2}{2m}$

(3) $\sigma = N\sqrt{\eta}\,\nu_{collision} \stackrel{def}{=} N\frac{L}{k_BT_\vartheta}$ ....

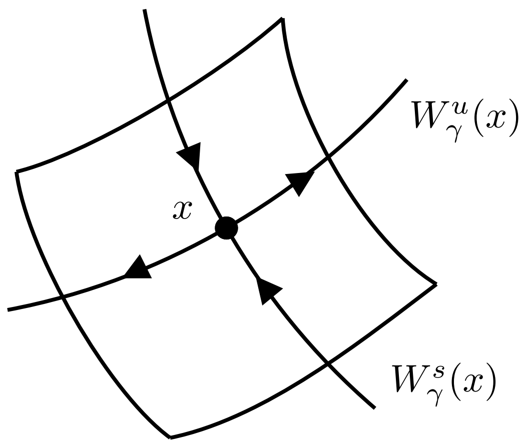
In general $\sigma = N\sum \underline{p}_i\cdot\partial_{\underline{p}_i}\underline{F}_i \stackrel{def}{=} \frac{\sum \underline{F}_i\cdot\dot{\underline{x}}_i}{k_BT_\vartheta}$

Thermostats (1), (3) are irreversible while (2) is reversible *i.e.* it generates a dynamics S_tx such that $IS_t = S_{-t}I$ wih $I(p,x) \stackrel{def}{=} (-p,x)$.

One says that motion *has a well defined statistics* μ if for all F smooth

$$\frac{1}{T}\sum_{n=0}^{T-1} F(S^n x)\xrightarrow[T\to\infty]{} \int \mu(dy)\,F(y) \quad \text{for (a.s.) all } x$$

Assumption: (*Chaotic hypothesis* (M,S) is such that
(1) *covariant*: $S\partial W^i_x = \partial W^i_{Sx}$, $i=u,s$; *continuous*: ∂W^i_x depends continuously on x
(2) *hyperbolic*:
(3) *transitivity*: there is a point with a dense orbit in phase space M under S



(Ruelle 73, Cohen, G, 95)

Consequence: a.a. initial data x have statistics μ independent on x: SRB–statistics

In equilibrium: $\Rightarrow$ ergodicity $\Rightarrow$ statistical mechanics

For instance: in the conservative case the stationary states are characterized by two parameters U,V: $\mu=\mu_{U,V}$. And *Boltzmann's heat theorem* follows

Let $p(U,V)$ be the $\mu_{U,V}$ average momentum transfer to walls

Let $T(U,V)$ be the $\mu_{U,V}$ average kinetic energy

Then $\frac{dU+p(U,V)dV}{T}$ = exact (hence = dS): **a parameterless universal relation**

Are there such consequences in nonequlibrium? when the chaotic hypothesis becomes the chaotic hypothesis?

A "*nonequilibrium ensemble*" is a collection of probability distributions on phase space which are stationary and are parameterized by macroscopic parameters like U, V, E in the example and by the thermostat force.

Experimentally discovered property (Evans,Cohen,Morriss, 93) in nunerical study of a *reversible* system of 54 particles. Define the observable

$$\frac{1}{\tau}\int_{-\tau/2}^{\tau/2}\frac{\sigma(S_t x)}{\sigma_+}\stackrel{def}{=}p(x)$$

has probability of being between p and $p+dp$ proportional to $e^{-\tau\zeta(p)+\ldots}$ and $\zeta(p)$ verifies the "Fluctuation Relation"

$$\zeta(-p)=\zeta(p)-p\sigma_+ \qquad (\text{“FR”})$$

This is a theorem in systems verifying the chaotic hypothesis (Cohen,G, 95).

Several experimental (numerical) checks

Nonnumerical tests attempted but, so far, not successfully (difficulty of observing such large fluctuations)

Lyapunov spectra and nonequilibrium ensembles equivalence in 2D fluid mechanics

L Rondoni, E Segre, & G G

DIMAT-Politecnico-Torino and Fisica-Roma1

NS and GNS equations ($d=2$ *Geometry*):

2D (or 3D) NS equations (dimensionless): *periodic geometry*, container side $L=2\pi$, viscosity $\nu=1$, Reynolds # R (large)

$\dot{\mathbf{u}}+R^2(\mathbf{u}\cdot\partial)\mathbf{u}=\Delta\mathbf{u}+\mathbf{f}-\partial p\ ,\quad \underline{\partial}\cdot\mathbf{u}=0,\qquad\quad \underline{f}=\cos\mathbf{k}_f\cdot\mathbf{x}$

when $R\to\infty$ motion becomes chaotic ($2D$ a value of $R^2>100$ is already sufficient).

Motions have a statistics $\mu_{1,R}$ (the SRB statistics, a probability distribution)

$$\frac{1}{T}\int_0^T F(S_t\mathbf{u})dt\to\mu_{1,R}(F)=\int\mu(d\mathbf{u})\,F(\mathbf{u})$$

Alternative equation: Euler + constraint that $\int\mathbf{u}^2=$ *const* + *effort function* $\mathbf{G}_1\overset{def}{=}\big(\Delta^{-1}(\mathbf{a}-\mathbf{f}-\partial p),(\mathbf{a}-\mathbf{f}-\partial p)\big)$.

(GNS): $\quad\dot{\mathbf{u}}+R^2(\mathbf{u}\cdot\partial)\mathbf{u}=\alpha(\mathbf{u})\,\Delta\mathbf{u}+\mathbf{f}-\partial p\ ,\quad \partial\cdot\mathbf{u}=0$

$$\alpha(\mathbf{u})=\frac{\int\underline{f}\cdot\mathbf{u}}{\int\mathbf{u}^2}$$

The SRB statistics of GNS is $m_{U,R}$.
NS does not conserve (kinetic) energy U. GNS does
NS is "irreversible", GNS is "reversible" (time reversal: $I\mathbf{u}=-\mathbf{u}\ \Rightarrow\ IS_t=S_{-t}I$)

Suppose that
NS–average of energy $=\ U$, GNS–energy $=\ U$
NS-statistics is $\mu_{1,R}$, GNS–statistics is $m_{U,R}$

Is there a relation between $\mu_{1,R}$ and $m_{U,R}$?

If $F(\mathbf{u}) > 0$ is "local": $F(\mathbf{u}) = \varphi(\{\mathbf{u_k}\}_{|\mathbf{k}|<n})$ (locality in Fourier space) then

$$\lim_{R\to\infty} \frac{\langle F\rangle_{\mu_{1,R}}}{\langle F\rangle_{m_{U,R}}} = 1, \qquad \textit{if} \qquad \mu_{1,R}(\frac{1}{2}\int \mathbf{u}^2) = U$$

R	$\sim$	volume
ν	$\sim$	temperature
U	$\sim$	energy
$R\to\infty$	$\sim$	thermodynamic limit

Analogy with equivalence of ensembles: can be tested numerically?

Tests are difficult (severe truncations)

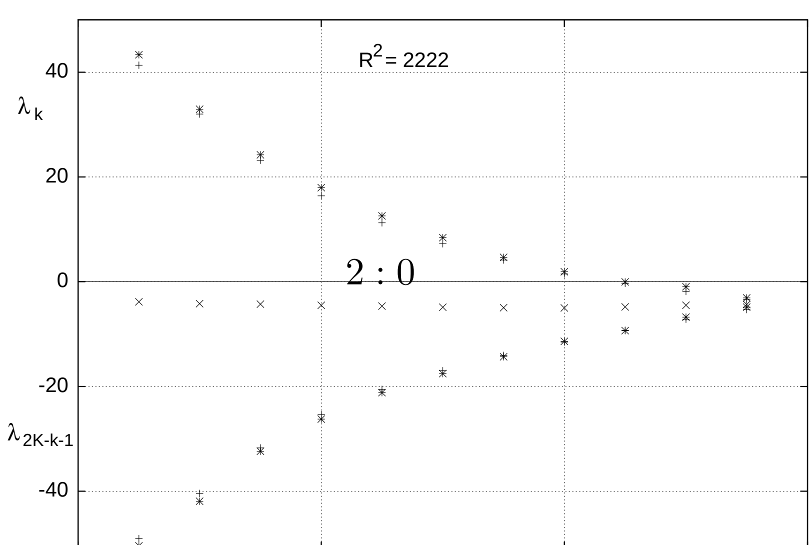
Rondoni–Segre (Nonlinearity 1999) perform various tests.

We attempted to study

1) whether the equivalence extends beyond the original formulation and one can identify even the Lyapunov spectrum of the two equations

2) given the equivalence we study the NS equation and try to see whether a part of the fluid behaves like the entire sample and we look at the *fluctuation relation* in a smaller portion of the fluid. This is necessary in order to compare with certain experiments that are being attempted or planned ([CL][G]). In macroscopic systems one can only hope to see important fluctuations if one examines small portions of the systems (analogy with density fluctuations in equilibrium)

Results on the Lyapunov exponents



Lyapunov spectra for NS with normal viscosity ($N = 5$ truncation) at $R^2 = 2222$ (left) and $R^2 = 5000$ (right), and corresponding GNS runs with constrained energy Q_0. The $2K - 2$ nontrivial exponents are drawn by associating each value of the abscissa $k = 1, 2, \ldots, K-1$ with the k–th largest exponent λ_k and the k–th smallest exponent $\lambda'_k = \lambda_{2K-k-1}$. Symbols
"+" $\rightarrow$ NS spectra,
"$*$" $\rightarrow$ GNS spectra,
"$\times$" to the sums $(\lambda_k + \lambda'_k)/2$ (NS case).
No "pairing" of exponents to a common average value, *unlike the cases of isokinetic Gaussian systems [DM96].*

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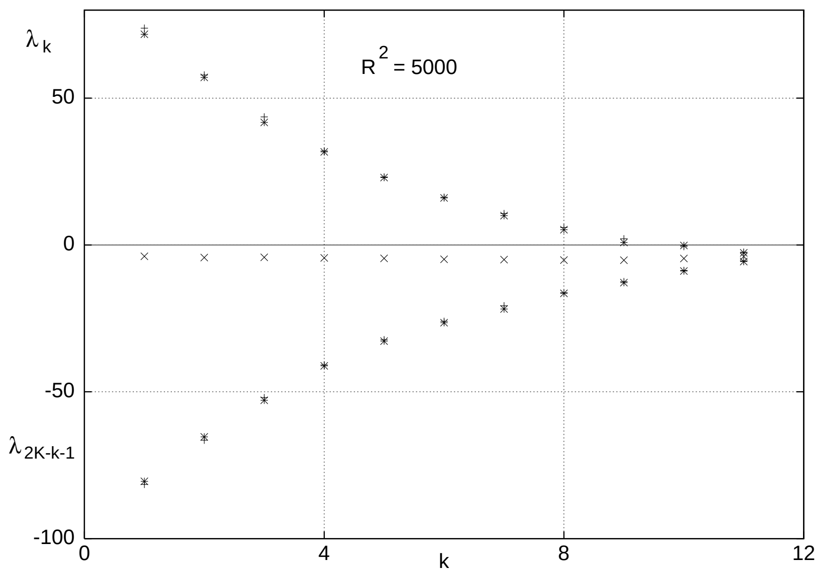

An attempt to check equivalence on systems with many more modes yields the following result

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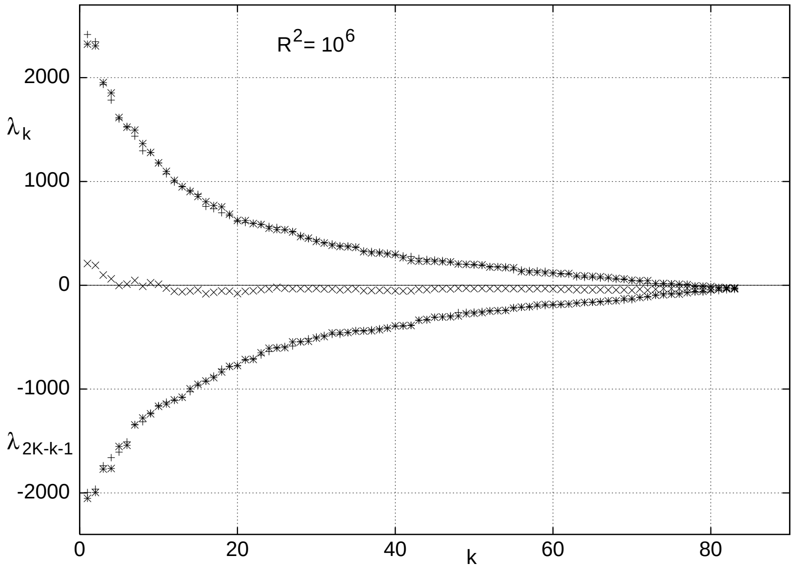

Lyapunov exponents $[N = 7, R^2 = 10^6$, and forcing modes $(4, -3), (3, -4)]$.
All $2K - 2 = 164$ nontrivial exponents are drawn as in Fig.1.
$(+)$ NS exponents
$(\times) \rightarrow$ graph of $(\lambda_k + \lambda'_k)/2$ (NS only)
$(*) \rightarrow$ corresponding GNS runs with fixed energy $(*)$ *i.e.* $m = 0, \ell = 1$
Error bars identified with the size of the symbols.
units of $1/\lambda_{max}$, λ_{max} being the largest Lyapunov exponent; runs of length $T \in [125, 250]$.
Overlap reflects the possible validity of the extension of the EC to the whole spectrum and to different members of the hierarchy of equations.

R^2	$\delta Q_0/\langle Q_0\rangle_{NS}$	$\triangle\alpha$	$\triangle Q_1$	$o(M)/M$
800	0.005	0.030	0.053	0.068
1250	0.020	0.018	0.062	0.057
2222	0.002	0.039	0.058	0.077
4444	0.050	0.021	0.093	0.059
5000	0.010	0.008	0.058	0.033

Equivalence of NS and GNS dynamics, i.e. with $\ell = 1$ and $m = 0$, for different Reynolds numbers. The last column gives the relative difference of the computed sums of the NS and GNS Lyapunov exponents, cfr. [GNStoNS]).

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