Friction, reversibility and nonequilibrium ensembles

Part of the recent progress has been due to

(a) Focus on stationary states out of equilibrium, [1].

(b) Modeling thermostats in terms of finite systems, [2, 3, 4], and deterministic equations.

Finite thermostats have been essential to clarify that reversibility and dissipation are not to be identified.

Thermostats $\Rightarrow$ Equations of motion: NOT Hamiltonian $\Rightarrow$ phase space contraction

BUT Time reversal is a fundamental symmetry while friction is phenomenological.

Hence the question arose, since Maxwell and Boltzmann, of which is the meaning of the phenomenological constants describing friction, [5, 6, 7], and more generally dissipation..

One can investigate, here in the paradigmatic case of the NS, equations whether

Every (even if macroscopic) dissipative evolution can be equivalent to a reversible one, provided motions are sufficiently chaotic, (usually are under large forcing or N).

This generates a proposal for a general theory of equivalence between statistical descriptions of stationary states as an extension of the theory of equilibrium ensembles to nonequilibrium. [8, 9, 10], inspired by the ideas on chaos, of Ruelle and Sinai, [11, 12].

$\Rightarrow$ *"In microscopically reversible (chaotic) systems time reversal symmetry cannot be spontaneously broken, but only phenomenologically so"*,[13].

Begin by defining "an ensemble $\mathcal{E}^c$" of probab. distrib. for NS2D equation in a periodic box of size $L = 1$ and subject to a fix (large scale) force $\vec{g}$, $\|\vec{g}\|_2 = 1$,*e.g.* **only** $g_{\pm(2,-1)} \neq 0$

for a velocity field $\vec{u}(\mathbf{x})=\sum_{\mathbf{k}}\vec{u}_{\mathbf{k}}e^{-2\pi\, i\,\mathbf{k}\cdot\mathbf{x}}$, $\vec{u}_{\mathbf{k}}=\overline{\vec{u}}_{-\mathbf{k}}$:

$$\dot{\vec{u}}+(\vec{u}\cdot\boldsymbol{\partial})\vec{u}=-\boldsymbol{\partial}p+\vec{g}+\nu\Delta\vec{u},\qquad \boldsymbol{\partial}\cdot\vec{u}=0 \qquad (*)$$

The only parameter here is ν and Reynolds # is $R=\frac{1}{\nu}$.

Hence as ν varies the motion defines stationary states $\boldsymbol{\mu}_\nu^C$ whose collection forms the *viscosity ensemble* $\mathcal{E}^c$

Conjecture: if interested in large scale observables, *i.e.* observables depending only on the $\vec{u}_{\mathbf{k}}$ with $|\mathbf{k}|<K$ for some arbitrary K then, in strongly chaotic regimes (*i.e.* R large enough), there *should be other ensembles* of distrib. which attribute same probability to K-local observables.

Mechanism: "same" as that for equilibrium ensembles in SM, *i.e.* special collections of stationary states with K playing the role of the finite volume and the truncation of the equation to $|\mathbf{k}|<V$ playing the role, as $V\to\infty$, of the thermodynamic limit (and $\nu\to 0$ the 0 temperature limit).

In the case of the NS equations **one** alternative ensemble here will be the family of stationary states for the equation

$$\dot{\vec{u}} + (\vec{u}\cdot\boldsymbol{\partial})\vec{u} = -\boldsymbol{\partial} p + \vec{g} + \alpha(\vec{u})\Delta\vec{u}, \qquad \boldsymbol{\partial}\cdot\vec{u} = 0 \qquad (**)$$

$$\alpha(\vec{u}) \stackrel{def}{=} \frac{\sum_{\vec{k}} \vec{k}^2\, \vec{g}_{\vec{k}}\cdot\vec{u}_{-\vec{k}}}{\sum_{\vec{k}} \vec{k}^4 |\vec{u}_{\vec{k}}|^2},$$

which have α so defined that the "dissipation" observable $\mathcal{D}(\tilde{\mathbf{u}}) = \int(\partial\tilde{\mathbf{u}}(\mathbf{x}))^{\mathbf{2}}\mathbf{dx}$ is an exact constant of motion.

Call $\alpha(\vec{u})$ a *"reversible viscosity"* (*because the equations are time reversible* and dissipative)

Denote $\boldsymbol{\mu}^M_{En}$ the stationary distr. describing statistical properties of stationary states of new equ. with $\mathcal{D}(\vec{u}) = En$.

We have now two "ensembles", *i.e.* collections of stationary distributions, namely

(1): Vary ν and let $\boldsymbol{\mu}_\nu^C$ stationary distrib. for **(*)** (NS2D). Let

$$\mathcal{E} = \boldsymbol{\mu}_\nu^C\Big(\int(\boldsymbol{\partial}\vec{u})^2\Big) = \boldsymbol{\mu}_\nu^C(\mathcal{D}(\vec{u}))$$

Their collection is an "ensemble" (viscosity ensemble), [∼canonical], of distr. parameterized by $\nu = \frac{1}{R}$

(2): Next consider the new equation **(**)**: it has $\mathcal{D}(\vec{u}) = \int(\boldsymbol{\partial}\vec{u})^2$ as exact constant of motion

Vary $\mathcal{E} \equiv \mathcal{D}(\vec{u})$ and let $\boldsymbol{\mu}_\mathcal{E}^M$ station. distrib.:

$$\nu = \boldsymbol{\mu}_\mathcal{E}^M(\alpha(\vec{u}))$$

and obtain a collection of distr. parameterized by $\mathcal{E}$: this is the (enstrophy ensemble), [∼microcanonical].

State $\boldsymbol{\mu}^M_{\mathcal{E}}$ labeled by $\mathcal{E}$ corresponds to state $\boldsymbol{\mu}^C_\nu$ labeled by ν $\Rightarrow$ and are equivalent, denoted $\boldsymbol{\mu}^C_\nu \sim \boldsymbol{\mu}^M_{\mathcal{E}}$, if i) **OR** ii) hold

$$i)\ \mathcal{E} = \boldsymbol{\mu}^C_\nu(\mathcal{D}(\cdot))$$
$$ii)\ \nu = \boldsymbol{\mu}^M_{\mathcal{E}}(\alpha(\cdot))$$

in the sense that they give the same statistics in the limit of large chaos to observables F which are "local observables": *i.e.* depend on finitely many Fourier comp. of $\vec{u}$.

Analogy: "canonical" $\boldsymbol{\mu}^C_\beta$ = "microcanonical" $\boldsymbol{\mu}^M_{\mathcal{E}}$.

Why? *e.g.* chaoticity implies self averaging for the observable $\alpha(\mathbf{u})$ which replaces viscosity in **(**)**:

$$\alpha(\mathbf{u}) = \frac{\sum_{\mathbf{k}} \vec{g}_{\mathbf{k}} \cdot \mathbf{u}_{-\mathbf{k}}}{\sum_{\mathbf{k}} |\vec{u}_{\mathbf{k}}|^2} \qquad \text{“self − averaging''} \text{ to } \qquad \nu$$

Problem: can reversibility be detected even in irrev. NS?

A theoretical basis can be searched in the "Chaotic hypothesis" (GC)

Chaotic hypothesis: "think of it as an Anosov system" (Cohen,G, if R is large), [14, 15, 11]

which is analogous to the periodicity≡ergodicity hypothesis of Boltzmann, Clausius, Maxwell, and possibly as unintuitive, [16, 17, 18].

Then in the reversible cases the phase space contraction rate $\sigma(\mathbf{u}) \stackrel{def}{=} \mathrm{div}\Big(\alpha(\mathbf{u})\Delta\mathbf{u}\Big)$ averaged over a time τ

$$p \stackrel{def}{=} \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{u}(t)}{\langle\,\sigma(\cdot)\,\rangle dt} \qquad (FT)$$

should have a PDF obeying a fluctuation relation, FR, [19].

This means that for large τ the probability distribution of p in $\boldsymbol{\mu}_{\mathcal{E}}^M$ (reversible viscosity ensemble) should fulfill, for some κ (see [9, 20]).

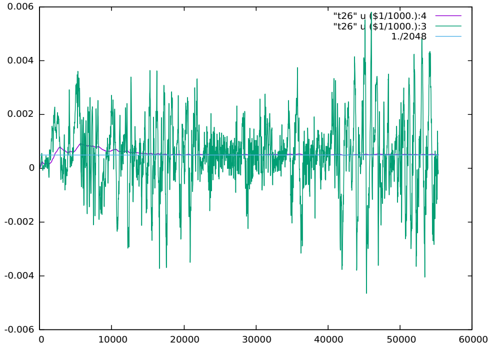
$$\frac{Prob_\tau(p)}{Prob_\tau(-p)} = e^{\tau\kappa\langle\,\sigma\,\rangle p+o(\tau)}, \qquad \tau \to \infty \qquad (\mathbf{FR})$$

Equivalence conjecture applied to the reversible viscosity ensemble $\boldsymbol{\mu}_{\mathcal{E}}^M$ and to the observable $\sigma(\mathbf{u})$ (which is not constant) would imply that $\sigma(\mathbf{u})$ fluctuates according to FR (original one!) in the corresponding $\boldsymbol{\mu}_\nu^C$.

Of course consistency requires that the average

$$\mu_\nu^C(\alpha(\mathbf{u})) = \nu$$

The above "predictions" can be tested. And one can explore if the equivalence conjecture can be extended even to the Lyapunov spectrum (although the Lyapunov exponents, as well as $\sigma(\mathbf{u})$ are not local quantities).



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At 960 modes and $R = 2048$: the evolution of the observable "reversible viscosity": $\alpha(\mathbf{u}) = \dfrac{\sum |\mathbf{k}|^2 F_{\mathbf{k}} \overline{\mathbf{u}}_{\mathbf{k}}}{\sum |\mathbf{k}|^4 |\mathbf{u}_{\mathbf{k}}|^2}$

According to the equivalence the time average of α should be $\mathbf{\frac{1}{R}}$. Represents the fluctuating values of α at intervals of 10^4 steps (see below); the middle line is the running average of α (at intervals of 100 steps) and it converges to $\mathbf{\frac{1}{R}}$ (horiz. line).

The graph gives the values only every 1000 interaction steps (otherwise it would be just a black stain).

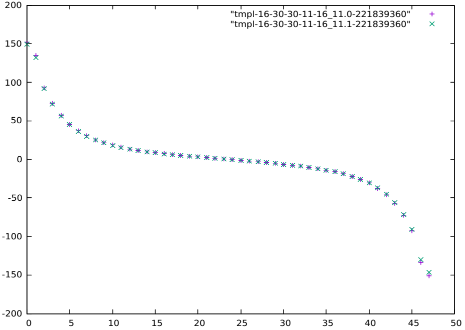
I stress that the experiments are carried using a truncated version of the NS2D eq. with cut-off at $|\mathbf{k}| < V$: the conjecture requires use of the non truncated equation, *i.e.* the limit $V \to \infty$, hence it can be tested only by trying to compare stability of results with increasing V and (so far the max V reached is $V = 961$, but the work is in progress).

We see that once the attractor might be considered reached, for instance if the running average of the reversible viscosity is close to $\frac{1}{R}$: however wild fluctuations remain and the statistics can be sampled to check whether the FR applies.

For comparing revers. and irrevers. Lyapunov spectra it should be necessary to compute a large number time steps.

This is being attempted: a few preliminary data follow

It is interesting to present a few recent (mostly preliminary) results (encouraging but which need further confirmation as they are not yet very stable).



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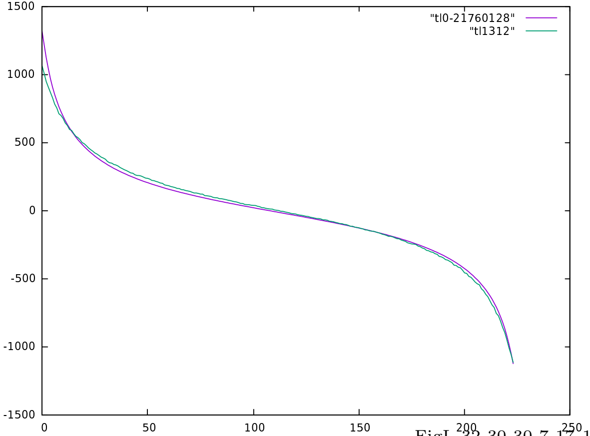
Local Lyapunov spectrum in a 48 modes truncation (7×7) of NS2D: $(+)=$ viscous, $(\times)=$ reversible and $R = 2048$.



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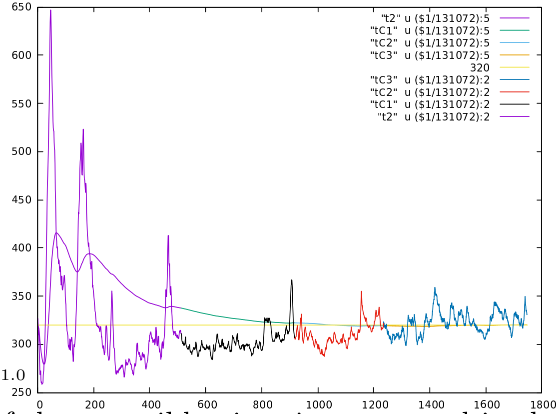
Graph of the Lyapunov spectra in a 15×15 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1) with (the 224 points) interpolated by lines, $R = 2048$. Preliminary

It is interesting to look at the fluctuations of En in the irreversible NS while the Lyapunov exponents of the previous image are measured: history (unit step 131072), running average and precomputed average of En



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The evolution of the reversible viscosity measured in the irreversible evolution has similar behavior.

Remarks: (1) The NS equations can be regarded, for large scale observables, as statistically equivalent to the motion of N microscopic particle subject to thermostats keeping for instance the total energy constant.

Then the microscopic motion is certainly chaotic at all R and this suggests that equivalence might hold at all R (even in the laminar regime or mildly chaotic flows where there may be several stationary states, [21]: a situation similar to the equivalence between ensembles in equilibrium and in presence of phase transitions).

In other words the equivalence for R large enough might extend to all R, (but the appropriate reversible models are likely to be different in the laminar regimes).

(2) The observable $\mathcal{D}(\vec{u})$ might not play a special role: it could be replaced by the energy $\int \vec{u}(x)^2 dx$. Some evidence for this has been found in [22] but doubts are raised in [23].

(3) And, **as in Statistical Mechanics**, it should be possible to fix more than a single observable thus generating many equivalent ensembles.

(4) The analysis applies word-by-word to NS3D: in that case it is even more interesting as there is a natural truncation at Kolmogorov scale. An important simulation, [4], has been performed on a 128^3 truncation of NS3D at scale $> O(R^{\frac{3}{4}})$ imposing many constraints: namely the energy content of **each shell** was fixed to the OK-value (following the $\frac{5}{3}$ power law) obtaining a stationary state (at high R) which on large scale observables is the same as the unconstrained evolution. See also [24].

(5) The conjecture here would say that fixing just one observable, namely the dissipation $\mathcal{D}(\mathbf{u})$, should be sufficient at large R for local observables statistics.

(6) A final remark: since the reversible viscosity model is reversible it is tempting to try to connect the fluctuations of the dissipation with the "fluctuation relation", [15, 9, 20]. This leads to think that
(a) another ensemble could be constructed replacing the viscosity with a whites Gaussian process, with average satisfying the fluctuation relation (?)
(b) the fluctuations of the reversible phase space contraction observed in the irreversible evolution should be a stochastic process obeying a fluctuation relation (see Fig. above): a further way to reveal reversibility in the irreversible evolution.

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Slides, edited, of the talk at the confrence
"Advances in Mathematics and Theoretical Physics", Roma, Accademia dei Lincei, 19-21 Sept. 2017.
on 19 Sept 2017.