Statistical ensembles for Navier-Stokes equation

Statistical properties of an Equilibrium state are obtained by several different probability distributions, *e.g.* canonical or microcanonical: which attribute the same average to physically interesting obervables. **Reminder**:

The probability distr. describing a system with ρV particles in volume V can be collected in families \mathcal{E}^{mc} , \mathcal{E}^{c} whose elements are parameterized by parameter E or, resp., β .

1) observables of interest are local observables $O \in \mathcal{O}_{loc}$: $O(\mathbf{p}, \mathbf{q})$ depending on \mathbf{p}, \mathbf{q} only through coordinates of particles $q_i \in \mathbf{q}$ with $q_i \in \Lambda$ where Λ is a volume $\ll V$

2) the probability distribution $\mu_{\beta}^{V} \in \mathcal{E}^{c}$ and $\widetilde{\mu}_{E}^{V} \in \mathcal{E}^{mc}$ are **correspondent** if β, E are s.t.

 $\mu_{\beta}^{V}(H_{V}(\mathbf{p},\mathbf{q})) = E$

Then

 $\lim_{V \to \infty} \mu_{\beta}^{V}(O) = \lim_{V \to \infty} \widetilde{\mu}_{E}^{V}(O)$

and μ 's are *equivalent* in the thermodynamic limit.

In case of phase transitions extra labels $\gamma, \tilde{\gamma}$ are added to identify the extremal distributions and it is possible to establish a correspondence between the extra labels $\gamma \longleftrightarrow \tilde{\gamma}$ so that the equivalence can be equally formulated.

Is it possible a similar description of the stationary states of nonequilibrium systems?

Think of a system whose evolution is described by an evolution eq. of u on a "phase space" M depending on a parameter R:

$\dot{u} = f_R(u)$

Typically eq. will be difficult and even existence-1-qness will be open problems.

For instance consider a system of infinitely many hard spheres of given density or an incompressible 3D NS fluid with periodic b.c.

Therefore the eq. will have to be regularized in $f_R^V(u)$ where V is a regularization parameter.

E.g. in stat. mechanics V is typically the container size: and the problem becomes finding the observables whose averages have a limit as $V \to \infty$. They exist and are O(u)which only depend on the points of u in a region $K \ll V$, local observables.

For the NS equation the regularization parameter could be a "UV cut-off" N. And it is natural to consider as observables whose average admit a limit as $N \to \infty$ the O(u) which only depend on the Fourier's components **k** of u ith $|\mathbf{k}| < K \ll N$. Once the class of observables is restricted it is to be expected (?) that several equations of motion could describe the stationary states of the same system.

E.g. the h.c. system can be described by the Hamilton eq.s but also by the isothermal equations

$$\dot{\mathbf{q}} = \mathbf{p}, \qquad \dot{\mathbf{p}} = -\partial_{\mathbf{q}}V(\mathbf{q}) - \alpha(\mathbf{p}, \mathbf{q})\mathbf{p}$$

where $\alpha(\mathbf{p}, \mathbf{q})$ is a multiplier which imposes $T(\mathbf{p}) = const$.

The stationary states of the two equations will be parameterized by the energy E or by the kinetic energy T; stationary states will be resp. $\delta(H(\mathbf{p}, \mathbf{q}) - E)d\mathbf{p}d\mathbf{q}$ or

$$e^{-\beta_0 V(\mathbf{q})} \delta(T(\mathbf{p}) - N\beta^{-1}) d\mathbf{p} d\mathbf{q}, \qquad \beta_0 = \beta (1 - \frac{1}{3N})$$

Interesting cases arise when the system is described by equations which obey a symmetry but they are phenomenologically described by non symmetric equations (cases of spontaneously broken symmetry).

Consider, as a typical case, the Navier-Stokes equation: in the case of the above incompressible fluid they can be regarded as Euler equations subject to a thermostat absorbing the heat due to the viscosity: which turns the equations into time-reversal breaking ones.

A paradigmatic case is a fluid in a periodic container 2/3-Dim., incompressible, **at fixed forcing** F (smooth, $||F||_2 = 1$) and kept at const. temp. by a thermostat. to dissipate heat via the force due to viscosity $\nu = \frac{1}{R}$ (consistently with incompressibility).

$$\begin{split} NS_{irr} &: \dot{u}_{\alpha} = -(\vec{u} \cdot \boldsymbol{\partial}) u_{\alpha} - \partial_{\alpha} p + \frac{1}{R} \Delta u_{\alpha} + F_{\alpha}, \qquad \partial_{\alpha} u_{\alpha} = 0 \\ \text{Velocity:} \quad \vec{u}(x) = \sum_{\vec{k} \neq \vec{0}} u_{\mathbf{k}} \frac{i\mathbf{k}^{\perp}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \overline{u}_{\mathbf{k}} = u_{-\mathbf{k}} \quad (\text{NS-2D}) \\ NS_{2,irr} &: \quad \dot{u}_{\mathbf{k}} = \sum_{\mathbf{k}_{1} + \mathbf{k}_{2} = \mathbf{k}} \frac{(\mathbf{k}_{1}^{\perp} \cdot \mathbf{k}_{2})(\mathbf{k}_{2}^{2} - \mathbf{k}_{1}^{2})}{2|\mathbf{k}_{1}||\mathbf{k}_{2}||\mathbf{k}|} u_{\mathbf{k}_{1}} u_{\mathbf{k}_{2}} - \nu \mathbf{k}^{2} u_{\mathbf{k}} + f_{\mathbf{k}} \end{split}$$

Immagine to truncate eq. supposing $|\mathbf{k}_j| \leq V$. Cut-off UV, V, is temporarily fixed (**BUT interest is on** $V \to \infty$).

NS 2D becomes an ODE in a phase space M_V with 4V(V+1) dimen. (In 3D $O(8V^3)$). Exist. & 1-ness trivial at D = 2, 3.

Remark that the map $Iu_{\alpha} = -u_{\alpha}$ implies $IS_t \neq S_{-t}I$, \Rightarrow : irreversibility.

Given init. data u, evolution $t \to S_t u$ generates a steady state (*i.e.* a probability distr.) $\mu_B^{irr,V}$ on M_V .

Suppose $\mu_R^{irr,V}$ unique aside a volume 0 of *u*'s, for simplicity. As *R* varies the steady distr. $\mu_R^{irr,V}(du)$ form a collection $\mathcal{E}^{irr,V}$: to be named

the statistical ensemble of stationary nonequilibrium distrib. for NS_{irr} .

And average energy E_R , average dissipation En_R , Lyapunov spectra (local and global) ... will be defined, e.g.: $E_R = \int_{M_V} \mu_R^{irr,V}(du) ||u||_2^2$, $En_R = \int_{M_V} \mu_R^{irr,V}(du) ||\mathbf{k}u||_2^2$

Consider new equation, NS_{rev} :

$$\dot{\mathbf{u}}_{\mathbf{k}} = \sum_{\mathbf{k_1}+\mathbf{k_2}=\mathbf{k}} rac{(\mathbf{k}_1^{\perp} \cdot \mathbf{k_2})(\mathbf{k}_2^2 - \mathbf{k}_1^2)}{2|\mathbf{k_1}||\mathbf{k_2}||\mathbf{k}|} \mathbf{u}_{\mathbf{k_1}} \mathbf{u}_{\mathbf{k_2}} - lpha(\mathbf{u})\mathbf{k}^2 \mathbf{u}_{\mathbf{k}} + f_{\mathbf{k}}$$

with α such t. $En(u) = ||\mathbf{k}u||_2^2$ is exact const of motion:

$$\alpha(u) = \frac{\sum_{\mathbf{k}} \mathbf{k}^2 F_{-\mathbf{k}} u_{\mathbf{k}}}{\sum_{\mathbf{k}} \mathbf{k}^4 |u_{\mathbf{k}}|^2} \qquad e.g. \ D = 2$$

The new equation keeps $\nu \sum_{\mathbf{k}} |\mathbf{k}|^2 |\mathbf{u}_{\mathbf{k}}|^2 = \nu \cdot enstrophy$ exactly constant

New eq. is reversible: $IS_t u = S_{-t}Iu$ (as α is odd).

 α is "a reversible viscosity"; (if $D = 3 \alpha$ is ~different)

Can be considered as model of "thermostat" acting on the fluid and should (?) have same effect of constant friction.

Evolution NS_{rev} generates a family of steady states $\mathcal{E}^{rev,V}$ on M_V : $\mu_{En}^{rev,V}$ parameterized by the constant value of enstrophy $En = \sum_{\mathbf{k}} |\mathbf{k}|^2 |u_{\mathbf{k}}|^2$.

 $\alpha(u)$ in NS_{rev} will wildly fluctuate at large R (*i.e.* small viscosity ν) thus "self averaging" to a const. value ν "homogenizing" the eq. into NS_{irr} with viscosity ν .

A first conjecture at small $\nu = \frac{1}{R}$ concerns the observables of large scale O, namely functions on the periodic container, *i.e.* functions O on M_V with Fourier's transform zero for $|\mathbf{k}| > K$, and K fixed.

The averages of large scale observables will tend to the same values as $R \to \infty$ for $\mu_R^{irr,V} \in \mathcal{E}^{irr,V}$ of NS_{irr} and for $\mu_{En}^{rev,V} \in \mathcal{E}^{rev,V}$ provided, $\mathcal{D}(\mathbf{u}) \stackrel{def}{=} \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2$ is s.t.

$$\mu_R^{irr,V}(\mathcal{D}) = En, \quad \text{or} \quad \mu_{En}^{rev,V}(\alpha) = \frac{1}{R}$$

Remark that multiplying the NS eq. by $\overline{u}_{\mathbf{k}}$ and sum on \mathbf{k} :

$$\frac{1}{2}\frac{d}{dt}\sum_{\mathbf{k}}|u_{\mathbf{k}}|^{2} = -\gamma \mathcal{D}(\mathbf{u}) + W(\mathbf{u}), \quad \gamma = \nu \text{ or } \alpha(\mathbf{u})$$

here $\mathcal{D}(\mathbf{u}) = \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2 = \text{enstrophy and}$ $W = \sum_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} \mathbf{u}_{-\mathbf{k}} = \text{work per unit time of the external force.}$

Hence time averaging

$$\frac{1}{R}\mu_R^{irr,V}(\mathcal{D}) = \mu_R^{irr,V}(W), \qquad \mu_{En}^{rev,V}(\alpha)En = \mu_{En}^{rev,V}(W)$$

But W is local (as **f** is such) and, if the conjecture holds, has equal average under the equivalence condition: hence $\mu_R^{irr,V}(\mathcal{D}) = En$ implies

$$\lim_{R \to \infty} R \mu_{En}^{rev,V}(\alpha) = 1$$

becoming a first rather stringent test of the conjecture.

More generally if O is a large scale observable it should be:

 $\mu_R^{irr,V}(O) = \mu_{En}^{rev,V}(O)(1 + o(1/R)) \quad \text{if} \quad \mu_R^{irr,V}(\mathcal{D}) = En$ But is $R \to \infty$, *i.e.* strong caos, necessary?

Here a particular feature of the NS equation becomes important.

Namely its being a scaling limit of a microscopic equation whose evolution is certainly chaotic and reversible.

Therefore NS is **different** from the many phenomenological and dissipative equations which are not directly related to fundamental equations.

For the latter cases strong chaos is **necessary** if a friction parameter is **changed** into a fluctuating quantity. There are many examples of phenomenological equations

- (1) (highly) truncated NS equations $(V < \infty \text{ fixed}), [1],$
- (2) NS with Ekman friction $(-\nu \vec{u} \text{ instead of } \nu \Delta \vec{u}), [2, 3],$
- (3) Lorenz96 model, [4],
- (4) Shell model of turbulence, (GOY), [5]

in such equations $R \to \infty$ is necessary: and, for each of them, it has been tested in few cases.

The NS_{irr} can be derived **if** $V = \infty$ from "first principles", (Maxwell, from molecular motion [6]). And microscopic motions are certainly chaotic.

There should not be conditions of developed chaos, not even when the motion is laminar.

Therefore consider the NS equations with UV cut-off V in dimension 2 or 3. The following conjecture emerges:

Large scale observables, *e.g.* O's depending only on $\mathbf{u}_{\mathbf{k}}$ with $|\mathbf{k}| < K$, (K arbitrary), have equal averages in the steady distr. in \mathcal{E}^{irr} and \mathcal{E}^{rev} obtained in the limit $V \to \infty$

$$\lim_{V \to \infty} \mu_{En}^{r,V}(O) = \lim_{V \to \infty} \mu_R^{i,V}(O)$$

provided $\mu_R^{i,V}(\mathcal{D}) = En$, which therefore implies $R\mu^{r,V}(\alpha) \xrightarrow[V \to \infty]{} = 1$ without requiring $R \to \infty$).

Analogy with equilibrium statistical mechanics is manifest

(a) The UV regularization (necessary if D = 3) V plays the role of the finite container volume

(b) K restricts to local observables

c) Reynolds R play role inverse canonical temperature β (*i.e.* viscosity $\nu \leftrightarrow$ temperature), while the dissipation (*i.e.* enstrophy) En the role of microcanonical energy.

But it will be useful to pause to illustrate a few prelimnary simulations and checks.

Unfortunately the simulations are in dimension 2 (D = 3 is at the moment beyond the available (to me) computational tools) although present day available NS codes should be perfectly capable to perform detailed checks in rapid time.

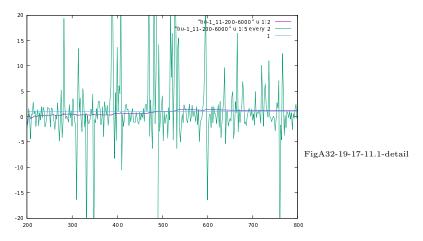


Fig.1-dettaglio: Running average of reversible friction $R\alpha(u) \equiv R \frac{2Re(f_{-\mathbf{k}_0} u_{\mathbf{k}_0})\mathbf{k}_0^2}{\sum_{\mathbf{k}} \mathbf{k}^4 |u_{\mathbf{k}}|^2}$, superposed to conjectured 1 and to the fluctuating values of $R\alpha(u)$. Initial transient is clear. Evol.: NS_{rev} , $\mathbf{R=2048}$, 224 modes, Lyap. $\simeq 2$, x-unit = 2^{19}

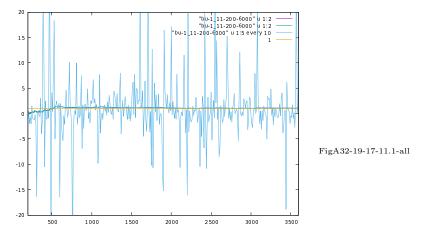


Fig.1: As previous fig. but time 8 times longer: data reported "every 10", or black.

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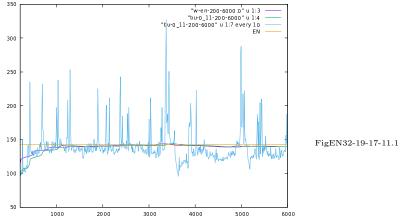


Fig.2: NS_{irr} : Running average of the work $R\sum_{\mathbf{k}} F_{-\mathbf{k}}u_{\mathbf{k}}|$ (violet) in NS_{rev} ; and convergence to average enstrophy En (orange straight line),

blue is running average of enstrophy $\sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$ in NS_{irr} , enstrophy **fluctuations** violet in NS_{irr} : **R=2048**.

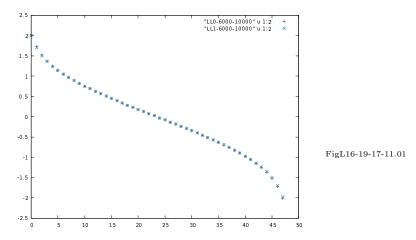


Fig.3: Spectrum (**local**) Lyapunov V=48 modes reversible & irreversible superposed; **R=2048**.

The difference can be made visible as:

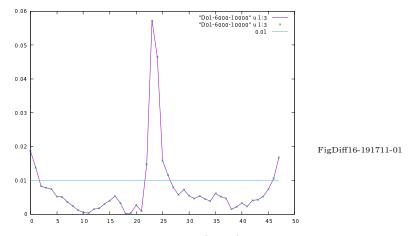


Fig.4: **Relative Difference** of (local) Lyap. exponents in Fig. preced. R=2048, 48 modes. Graph of $\frac{|\lambda_k^{rev} - \lambda_k^{irr}|}{\max(|\lambda_k^{rev}|, \lambda_k^{irr}|)}$; Level line marks 1%.

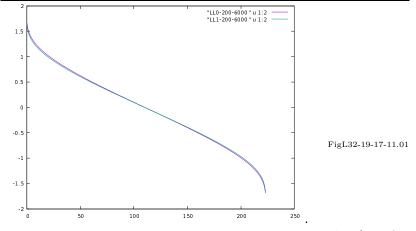


Fig.5: More Lyapunov spectrume in 15×15 modes (i.e. for NS2D rever. & irrev. R = 2048, 240 modes on 2^{13} steps. Spectra evalued every 2^{19} integr. steps. (and averaged over 200 samples).

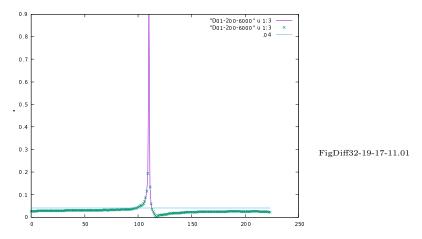
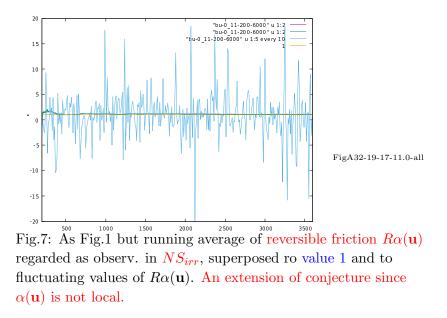


Fig.6: **Relative difference** of the (local) Lyapunov exp. of the preceding fig. 240 modes. The line is the 4% level.

The following Fig.7 (similar to Fig.1 but w. NS_{irr}):



The figure suggests (from the theory of Anosov systems): (1) **Check** the "Fluctuation Relation" in the **irreversible** evolution: for the divergence (trace of the Jacobian) $\boldsymbol{\sigma}(u) = -\sum_{\mathbf{k}} \partial_{u_{\mathbf{k}}}(\dot{u}_{\mathbf{k}})_{rev}$: let p (time τ average of $\frac{\sigma}{\langle \sigma \rangle}$)

$$p \stackrel{def}{=} \frac{1}{\tau} \int_0^\tau \frac{\boldsymbol{\sigma}(\mathbf{u}(t))}{\langle \boldsymbol{\sigma} \rangle_{irr}} dt,$$

then a theorem for Anosov systems:

$$\frac{P_{srb}(p)}{P_{srb}(-p)} = e^{\tau \mathbf{1} \mathbf{p} \langle \boldsymbol{\sigma} \rangle_{irr}} \text{ (sense of large deviat. as } \tau \to \infty)$$

it is a "reversibility test on the irreversible flow"

Anosov systems play the role, in chaotic dynamics that harmocic oscillators cover for ordered motions. They are a paradigm of chaos. The idea is based on **Sinai** (for Anosov syst.), **Ruelle**, **Bowen** (for Axioms A syst.), [7, 8, 9]

Attention on Anosov syst. leads to:

Chaotic hypothesis: An empirically chaotic evolution takes eventually place on a smooth surface \mathcal{A} , "attracting surface" in phase space and, on \mathcal{A} , the evolution (map S or flow S_t) is a Anosov syst.

It is a strict and general heuristic interpretation of the original ideas on turbulence phenomena, [9], see [10, endnote 18], [11, 12], [13].

BUT: various are the obstacles to its applicability and resolving them leads to new interesting problems.

Problem: if $\mathcal{A} \subset M_V$ e \mathcal{A} has lower dimension, the time reversal symmetry I cannot be applied because $I\mathcal{A} \neq \mathcal{A}$. This certainly occurs if V becaomes large enough, [14, 15].

However a further symmetry P may exist between \mathcal{A} and $I\mathcal{A}$ commuting with evolution S_t : $PS_t = S_t P$.

Then $P \circ I : \mathcal{A} \to \mathcal{A}$ becomes a time reversal symmetry of the motion restricted to \mathcal{A} . And there are geometrical conditions which in special cases guarantee existence of P("Axiom C" systems, [16]).

However even supposing existence of P, still is is not possible to apply FR because, at best, it would concern the contraction $\sigma_{\mathcal{A}}(\mathbf{u})$ of \mathcal{A} and not the $\sigma(\mathbf{u})$ of M_V .

The $\sigma(\mathbf{u})$ riceives contributions from the exponential approach to \mathcal{A} : which obviously do not contribute to $\sigma_{\mathcal{A}}$. How to recognize such contributions ?

Help could come from "pairing rule"

Often the Lyapunov exponents (local and global) arise in pairs with almost constant average or average on a regular curve.

In several systems the pairs have an exactly constant average.

An idea can be obtained from the local exponents (the eigenvalues of the simmetric part of the Jacobian matrix of the evolution). For instance in NS it is

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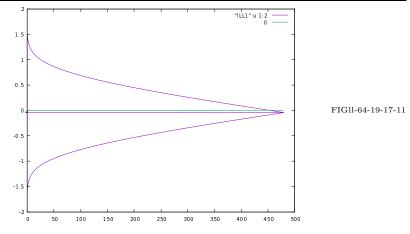
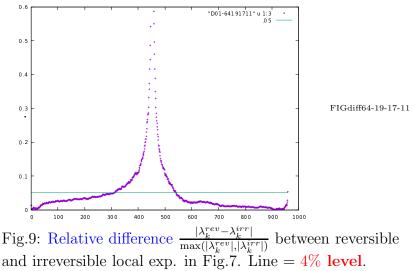


Fig.8: R = 2048, **960modes**, **local** exponents ordered decreasing: s.t. λ_k , $0 \le k < d/2$, and increasing λ_{d-k} , $0 \le k < d/2$, the line $\frac{1}{2}(\lambda_k + \lambda_{d-1-k})$ and the line $\equiv 0$. Irreversible case and apparent pairing rule

The graph of the reversible exponents is again almost superposed to the above and the following figure gives the relative difference of the 960 correponding exponents.



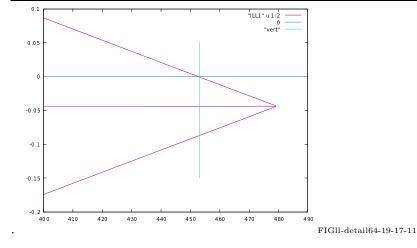


Fig.10: Detail of Fig.8 showing the NS_{irr} exponents and the line $\equiv 0$: it illustrates the "dimensional loss" $\sim \frac{450}{490}$. R = 2048, 960 modes.

The figures indicate:

(a) revers. and irrrev. exponents are very close: but this does not follow from the conject. (as the exponents are not local observables) \rightarrow suggests: possible equivalence for a larger class of observables.

(b) It has been proposed that the attracting surface \mathcal{A} has dimension = twice the number of positive exponents: which implies in cases of pairing that it is twice the number of pairs with opposite sign.

Implication: $\sigma_{\mathcal{A}}(\mathbf{u})$ is proportional to the total $\sigma(\mathbf{u})$ in the cases of pairing to a constant

$$\sigma_{\mathcal{A}}(\mathbf{u}) = \boldsymbol{\varphi}\sigma(\mathbf{u}), \qquad \boldsymbol{\varphi} = \frac{number\ of\ opposite\ pairs}{total\ number\ of\ pairs}$$

and in the case of pairing to a more general curve $\sigma_{\mathcal{A}}(u) = \sigma(u) + \sum_{pairs < 0} (\lambda_j + \lambda'_j)$. Why?

Idea: negative pairs correspond to the exponents associated with the attraction to \mathcal{A} : hence do not count for the computation of $\sigma_{\mathcal{A}}$.

The FR will hold, by the C.H., but with a slope $\varphi < 1$:

 $au p \boldsymbol{\varphi} \sigma$, rather than $au p \sigma$: in fig. $\boldsymbol{\varphi} \simeq \frac{450}{490}$

If true: this will be a check of reversibility in NS_{irr} .

IF FR holds, it is possible to think to one more statistical ensemble \mathcal{E}^{st} consisting in the stationary PDF's for NS_{st}

 $\dot{u}_{\alpha} = -(\vec{u} \cdot \partial)u_{\alpha} - \partial_{\alpha}p + \nu(u)\Delta u_{\alpha} + F_{\alpha}, \qquad \partial_{\alpha}u_{\alpha} = 0$

where $\nu(u)$ is a stochastic process (*e.g.* gaussian) uncorrelated but with average $\langle \nu \rangle = \frac{1}{R}$ and with a distribution respecting the FR (*i.e.* dispersion = average in the gaussian case).

More elaborate checks are being attempted:

(a) moments of large scale observables rev & irr

(b) local Lyap. exponents of other matrices different from the Jacobiank

(c) check of the fluctuation rel., particularly in the irrev. cases, which from the previous figures is shown to be accessible already with 960 modes and R = 2048: \Rightarrow FR with slope $\varphi < 1$ (Axiom C ?), [12, 11].

(d) More values of R and N an interesting example is Fig.10 with R much larger than in the preceding cases.

Example of moments of local observables:

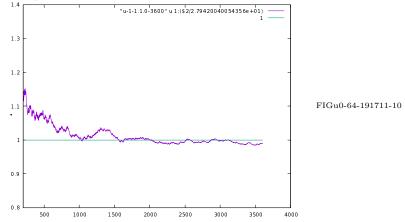
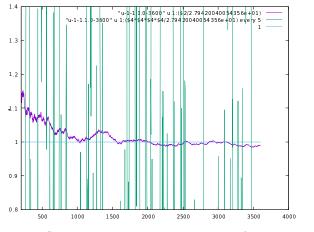


Fig.11: Running averages rev of $|Re u_{11}|^4 / \langle Re u_{11}|^4 \rangle_{irr}$, R = 2048, 224 modes. Conjecture yields ratio tending to 1

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FIGu1-64-191711-10

Fig.12: Same running averages rev of $|Re u_{11}|^4 / \langle Re u_{11}|^4 \rangle_{irr}$, for R = 2048, and their rev. fluctuations, 224 modes.

Finally a rigorous estimate of the number \mathcal{N} of Lyap. exp. (local and global ordered decreasing), needed so that their sum remains > 0:

$\leq \sqrt{2}A(2\pi)^2\sqrt{R}\sqrt{R\,En}, A=0.55..$

in dimension 2, while at dimension 3 a similar estimate holds but it involves a norm different from the enstrophy. (Ruelle if d = 3 and Lieb if d = 2, 3, [17, 15]. Applied here it would give $\mathcal{N} \sim 2.10^4$ for NS 2D: not accessible in the simulations presented here but not impossible in principle with available computers and computation methods already available, at least if D = 2.

Finally a warning that further careful checks are required, particularly because the inspiring ideas are, to say the least, **controversial** as shown by the following quote, selected among the several, from a well known treatise:

CH is dismissed (by many) with arguments like (1999)

'More recently Gallavotti and Cohen have emphasized the "nice" properties of Anosov systems. Rather than finding realistic Anosov examples they have instead promoted their "Chaotic Hypothesis": if a system behaved "like" a wildly unphysical but well-understood] time reversible Anosov system there would be simple and appealing consequences, of exactly the kind mentioned above. Whether or not speculations concerning such hypothetical Anosov systems are an aid or a hindrance to understanding seems to be an aesthetic question., [18].

Avoiding to comment on the statement I stress that Statistical Mechanics, from Clausius, Boltzmann and Maxwell has been a simple, surprising, consequence of the "[wildly unphysical but well-understood]" periodicity of the collective motions of 10¹⁹ gas molecules, [19].

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