Statistical ensembles out of equilibrium: turbulence

Equilibrium states $\Rightarrow \rho V$ particles in volume V and interaction potential $U(\mathbf{q}) \Rightarrow$ probability distributions determining average values of many observables

- 1) i.e. local observables $O \in \mathcal{O}_{loc}$: $O(\mathbf{p}, \mathbf{q})$, depend on $q_i \in \mathbf{q}$ located in regions $\Lambda \subset V$.
- 2) distributions depend on equations of motion.

Which among the invariant prob. distr. is the correct one? For isolated systems Ergodic Hypothesis (EH) provides (a) solution: for a.a. data $\mathbf{u} = (\mathbf{p}, \mathbf{q})$

$$\mu_E(d\mathbf{p}d\mathbf{q}) = \frac{1}{Z}\delta(H_V(\mathbf{p}, \mathbf{q}))d\mathbf{p}d\mathbf{q}$$

As the energy E = eV varies the distributions are collected in $\mathcal{E}_E^{mc,V}$, microcanonical ensemble.

Why? data are always generated randomly with a unknown distribution which however is (taciltly?) assumed of the form $\rho(\mathbf{u})d\mathbf{u}$.

Then if the system is chaotic (e.g. hyperbolic) it is a theorem that a.a data **u** evolve visiting sets with well defined frequency *independent* of the unknown distribution for the data generation, called the SRB distribution.

This asymptotic behavior only depends on the hyperbolicity of the motion on phase space or, in the case of dissipative evolution, on the attracting set.

The two remarks contain the essence of Ruelle's proposal:

"the initial data are random with distr, $\rho(\mathbf{u})d\mathbf{u}$ (unknown but absolutely cont.) and motions are "generically" chaotic so that the statistics of the motions is uniquely determined as the SRB distribution"

If account is taken that only few observables are physically interesting then other distributions might provide the same averages for the interesting observables, particularly in the case of macroscopic systems, and can be collected in other "ensembles" \mathcal{E}^V_β . For instance the canonical distrib.

$$\mu_{\beta}^{c,V}(d\mathbf{p}d\mathbf{q}) = \frac{1}{Z}e^{-\beta H_V(\mathbf{p},\mathbf{q})}d\mathbf{p}d\mathbf{q}$$

The apparent resulting ambiguity is solved, in equilibrium, by the equivalence between distrib. in $\mathcal{E}_E^{mc,V}$ and $\mathcal{E}_\beta^{c,V}$: "canonical distribution $\mu_\beta^V \in \mathcal{E}^c$ is equivalent to the microcanoical $\widetilde{\mu}_E^V \in \mathcal{E}^{mc}$ if β, E are s.t.

$$\mu_{\beta}^{V}(H_{V}(\mathbf{p},\mathbf{q})) = E \implies \lim_{V \to \infty} \mu_{\beta}^{V}(O) = \lim_{V \to \infty} \widetilde{\mu}_{E}^{V}(O)$$

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

Ruelle's generalization of the EH unifies equilibrium and nonequilibrium and assuming that generically chaotic systems are such in the precise sense of Axiom A it follows that also in nonequilibrium there is a unique statistics for the stationary states.

It is therefore natural to ask whether a theory of ensembles (i.e. of families of distr.) in 1-to-1 correspondence yield equivalent statistical descriptions for same stationary state.

Here the idea will be exploited in the simplified version adopted by Cohen and G replacing axiom A with the assumption that "generically" chaotic motions evolve towards a smooth attracting surface over which motion is chaotic in the sense of Anosov (stronger than Axiom A): named Chaotic hypothesis or CH.

In any theory of large (macroscopic) systems \rightarrow key points

- (1) Regularization of equations (via a "cut off")
- (2) Restriction on observables ("local observables")

Regularization, necessary in essentially all cases, replaces $\dot{\mathbf{u}} = f_R(\mathbf{u})$ (∞ -dim) by a regularized $\dot{\mathbf{u}} = f_R^V(\mathbf{u})$ ($< \infty$ -dim).

Stationary $\mu_R^V(d\mathbf{u})$ uniquely determined by Ruelle's extension of ergodic hypothesis (i.e. SRB distrib.).

Form a family \mathcal{E}_R^V of distributions assigning average values to the restricted observables. For instance:

- (a) In Stat. Mech: local observables and cut-off V = container size; \Rightarrow find their averages at limit as $V \rightarrow \infty$:
- (b) In Fluid Mech.: large scale observables (*i.e.* functions of velocities with "waves" $|\mathbf{k}| < K \ll N$) and cut-off N on the maximum wave $|\mathbf{k}|$: \Rightarrow find averages at limit as $N \to \infty$

Concentrate attention on the paradigmatic case of periodic NS fluid, $[1,\ 2],$

- (a) 2/3-Dim., incompressible,
- (b) fixed large scale forcing F (e.g. with only one or few Fourier's waves and $||F||_2 = 1$),
- (c) dissipate heat via viscosity $\nu = \frac{1}{R}$

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

$$\begin{array}{l} \textit{NS}_{2,\textit{irr}} \colon \, \dot{u}_{\mathbf{k}} = \sum_{\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}} \frac{(\mathbf{k}_1^{\perp} \cdot \mathbf{k}_2)(\mathbf{k}_2^2 - \mathbf{k}_1^2)}{2|\mathbf{k}_1||\mathbf{k}_2||\mathbf{k}|} u_{\mathbf{k}_1} u_{\mathbf{k}_2} - \nu \mathbf{k}^2 u_{\mathbf{k}} + f_{\mathbf{k}} \end{array}$$

$$Iu_{\alpha} = -u_{\alpha}$$
 implies $IS_t^{irr} \neq S_{-t}^{irr}I$, \Rightarrow : irreversibility.

"Regularize eq.": waves $|\mathbf{k}_i| \leq N$. At UV-Cut-off, N.

Given init. data u, evolution $u \to S_t^{irr}u$ generates a steady state (*i.e.* a SRB probability distr.) $\mu_R^{irr,N}$ on M_N .

Unique out a 0-volume of u's, for simplicity [AT R small: "NS gauge symmetry" exists.; phase transitions, [3, 4, 5].

As R varies steady distr. $\mu_R^{irr,N}(du)$ are collected in $\mathcal{E}^{irr,N}$:

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

Average energy E_R , average dissipation En_R , Lyapunov spectra (local and global) ... will be defined, e.g.:

$$E_R = \int_{M_N} \mu_R^{irr,N}(du)||u||_2^2, \qquad En_R = \int_{M_N} \mu_R^{irr,N}(du)||\mathbf{k}u||_2^2$$

Consider new equation, NS_{rev} (with cut-off N):

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

with α s. t. $\mathcal{D}(u) = ||\mathbf{k}u||_2^2 = En$ (the enstrophy)is exact const of motion on $u \to S_t^{rev}u$.:

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

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

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

Rev. eq. is an empirical model of "thermostat" on the fluid and should (?) have **same effect** of empirical constant friction (that can also be a thermostat model).

 NS_{rev} generates a family of steady states $\mathcal{E}^{rev,N}$ on M_N : $\mu_{En}^{rev,N}$ parameterized by constant value of **enstrophy** En.

 $\alpha(u)$ 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 .

Equivalence mechanism by analogy with Stat. Mech.

- (1) analog of "local observables": functions O(u) which depend only on $u_{\mathbf{k}}$ with $|\mathbf{k}| < K$. "Locality in momentum"
- (2) analog of "Volume": just the cut-off N confining the \mathbf{k}
- (3) analog of "state parameter": viscosity $\nu = \frac{1}{R}$ (irrev. case) or enstrophy En (rev. case).

Equivalence condition:
$$\mu_{En}^{rev,N}(\alpha) = \frac{1}{R}$$

Equivalence is **conjectured** at $N = \infty$ in analogy with the thermodynamic limit $V \to \infty$, for all R.

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

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

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

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

(transport terms = 0, D = 2, 3), $\mathcal{D}(\mathbf{u}) = \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2 =$ enstrophy and $W = \sum_{\mathbf{k}} \mathbf{f}_{\mathbf{k}} \mathbf{u}_{-\mathbf{k}} =$ power of external force.

Hence time averaging

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

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

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

This becomes a first rather stringent test of the conjecture.

Since the equivalence rests on the rapid fluctuations of $\alpha(u)$ a second idea is that if N is **kept finite** then, more generally, if O is a large scale observable it should be:

$$\mu_R^{irr,N}(O) = \mu_{En}^{rev,N}(O)(1+o(1/R)) \qquad \text{if} \qquad \mu_R^{irr,N}(\mathcal{D}) = En$$

So a parallel (different) idea arises: i.e. $N \to \infty$ and R fixed can be replaced by N fixed and $R \to \infty$.

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

Unfortunately the following 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, [6].

Concentrate on the first test:

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

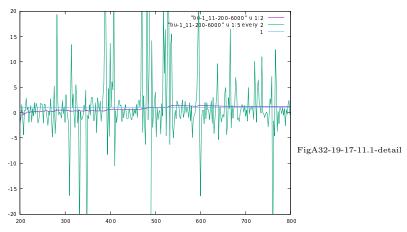


Fig.0 (detail): Running average of reversible friction $R\alpha(u) \equiv R \frac{2Re(f_{-\mathbf{k}_0}u_{\mathbf{k}_0})\mathbf{k}_0^2}{\sum_{\mathbf{k}}\mathbf{k}^4|u_{\mathbf{k}}|^2}$, superposed to conjectured 1 and to the fluctuating values of $R\alpha(u)$. **Initial transient** t < 800. Evol.: NS_{rev} , $\mathbf{R} = 2048$, 224 modes, Lyap. $\simeq 2$, x-unit $= 2^{19}$

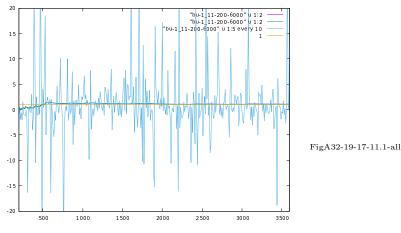


Fig.1: As previous fig. but time 8 times longer: data reported "every 10", or black.

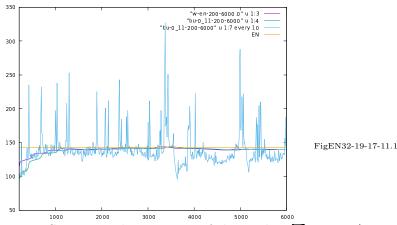


Fig.2: NS_{irr} : Running average of the work $R \sum_{\mathbf{k}} F_{-\mathbf{k}} u_{\mathbf{k}} |$ (violet) in NS_{rev} ; and convergence to average enstrophy En (orange straight line), blue is running average of enstrophy $\sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$ in NS_{irr} , enstrophy fluctuations violet in NS_{irr} : $\mathbf{R} = 2048$.

unexpected ?, [7]:

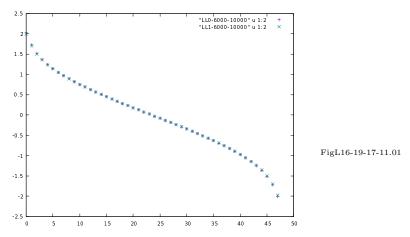


Fig.3: Spectrum (local) Lyapunov V=48 modes reversible & irreversible superposed; R=2048.

The difference can be made visible as:

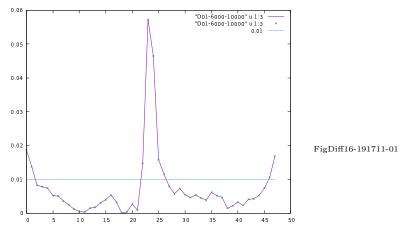


Fig.4: Relative Difference of (local) Lyap. exponents in Fig. preced. R=2048, 48 modes.

Graph of $\frac{|\lambda_k^{rev} - \lambda_k^{irr}|}{\max(|\lambda_k^{rev}|, \lambda_k^{irr}|)}$; Level line marks 1%.

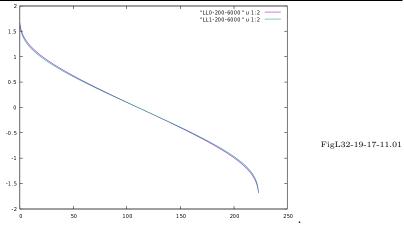


Fig.5: More local Lyapunov spectrum in 15×15 modes (i.e. for NS2D rever. & irrev. R = 2048, 240 modes on 2^{19} steps. Spectra evaluated every 4 time units. (and averaged over 200 samples).

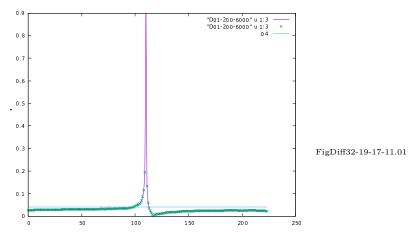
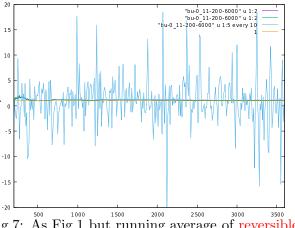


Fig.6: **Relative difference** of the (local) Lyapunov exp. of the preceding fig. 240 modes. The line is the 4% level.

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



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Fig.7: As Fig.1 but running average of reversible friction $R\alpha(\mathbf{u})$ regarded as observ. in NS_{irr} , superposed ro value 1 and to fluctuating values of $R\alpha(\mathbf{u})$. An extension? of conjecture since $\alpha(\mathbf{u})$ is not local.

The figure suggests (from the theory of Anosov systems):

Check the "Fluctuation Relation" in the irreversible evolution: for the divergence (trace of the Jacobian) $\sigma(u) = -\sum_{\mathbf{k}} \partial_{u_{\mathbf{k}}}(\dot{u}_{\mathbf{k}})_{rev}$: 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. Are NS Anosov systems?

The idea is based on **Sinai** (for Anosov syst.), **Ruelle**, **Bowen** (for Axioms A syst.),[8, 9, 10] *Chaotic hypothesis*.

Can this be applied to turbulence? However:

Problem 1: if attracting set \mathcal{A} has lower dimension, time reversal symmetry I cannot be applied because $I\mathcal{A} \neq \mathcal{A}$. This certainly occurs if N becomes large enough, [11, 12].

Help could come **if** exists further symmetry P between \mathcal{A} and $I\mathcal{A}$ commuting with 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, [13]).

Problem 2: 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 $\sigma(\mathbf{u})$ receives 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 Lyapunov exps (local and global) arise in pairs with almost constant average or average on a regular curve.

In a few systems pairs have an exactly constant average.

An idea can be obtained from the local exponents (eigenvalues of the symmetric part of the evolution Jacobian matrix).

For instance NS seems to enjoy a pairing rule:

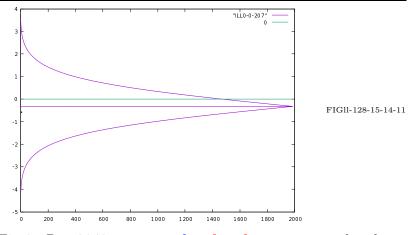


Fig.8: R = 2048, **3968modes**, **local** exponents ordered decreasing: s.t. λ_k , $0 \le k < d/2$, and increasing λ_{d-k} , $0 \le k < d/2$, the line $\frac{1}{2}(\lambda_k + \lambda_{d-1-k})$ and the line $\equiv 0$. Irreversible case and apparent pairing rule and dimensional loss $\varphi \simeq \frac{1500}{2000}$.

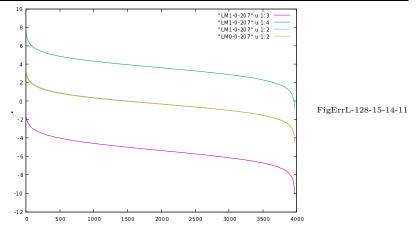


Fig.9: Fluct. max.-min. of Fig.5 showing the N = 3968 NS_{rev} -exponents average and max-min variation and the remarkable coincidence of with the NS_{irr} exponents (which show instead very small fluct.

The figures indicate:

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

(b) It has been proposed, [14, p.445],[7], that attracting surface \mathcal{A} dimension = twice the number of positive exponents: hence in cases of pairing it is twice num. of opposite sign pairs.

Implication: $\sigma_{\mathcal{A}}(\mathbf{u})$ is proportional to the total $\sigma(\mathbf{u})$ if 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 $\sigma_{\mathcal{A}}(u) = \sigma(u) + \sum_{pairs < 0} (\lambda_i + \lambda_i')$. 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 $\varphi < 1$:

$$au p oldsymbol{arphi} \sigma$$
, rather than $au p \sigma$: in fig. $oldsymbol{arphi} \simeq rac{450}{490}$

If true: this will be a "check of reversibility" in NS_{irr} . More elaborate checks are being attempted: [6, 15] +

- (a) moments of large scale observables rev & irr
- (b) local Lyap. exps of matrices different from Jacobian
- (c) check of the fluctuation rel., particularly in irrev. cases, (shown above to be accessible already with 960 modes and R = 2048): \Rightarrow FR with slope $\varphi < 1$ (Axiom C?), [14, 16].
- (d) More values of R and N an example with R larger than in the preceding cases yields similar results (not shown).

Example of moments of local observables:

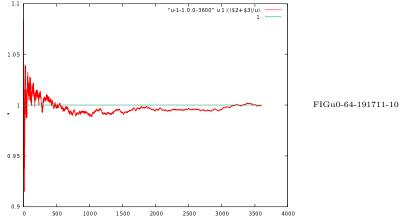
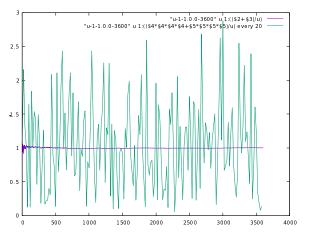


Fig.10: Running averages rev of $(|Re u_{11}|^4 + |Im u_{11}|^4)/\langle |Re u_{11}|^4 + |Im u_{11}|^4\rangle_{irr}, R = 2048,$ 960 modes. Conjecture yields ratio tending to 1



FIGu1-64-191711-10

Fig.11: Same running averages rev of $(|Re u_{11}|^4 + |Im u_{11}|^4)/\langle |Re u_{11}|^4 + |Im u_{11}|^4\rangle_{irr}$, for R = 2048, and their rev. fluctuations, 960 modes.

Concluding the simulation

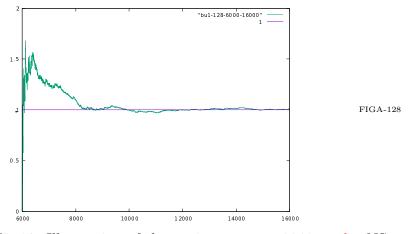


Fig.12: Illustration of the conjecture on a 3968 modes NS: the running average of $R\alpha$ in the reversible NS should tend to 1, according to conjecture.

Finally rigorous estimate of number \mathcal{N} of Lyap. exp. needed so that their sum remains > 0:

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

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, 12].

Applied here it would require $\mathcal{N} \sim 2.10^4$ 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 further careful checks are required, particularly since inspiring ideas are, to say the least, controversial as shown by quotes from a well known treatise, [18, p.344-347] and [2, app.A].

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Amherst, November 15 2019