Ireversibility and Statistical Ensembles in Nonequilibrium: Navier-Stokes example

Question: is it possible to extend the probabilistic representation of the equilibrium states to stationary states of dissipative systems?

?? In analogy with equilibrium it should be possible to find families of PDF's arising as stationary distributions for different evolutions which nevertheless attribute the same averages to large classes of observables.

Is dissipation an obstacle?: it generates irreversibility; violating time reversal. But time reversal I is a fundamental symmetry and "cannot" be spontaneously violated.

Hence also steady states of dissipative systems should be describable by reversible eq. of motion.

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 and 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.

Once a regularization is introduced, and the family of observables is limited, conceivably different equations could lead to the same results, at least in the limit $V \to \infty$:

$$\dot u = f_R^{i,V}(u) \quad \textbf{or} \quad \dot u = f_R^{r,V}(u) \quad \textbf{with} \quad f_R^{i,V} \neq f_R^{u,V}$$

Particularly if the equ. follows, *e.g.* via some (scaling) limit, from a more detailed descr.: which already provides a second representation.

And if the fundamental description is reversible there might be reversible equations leading to the the same stationary states, because a fundamental symmetry "cannot be lost".

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 due to viscosity $\boldsymbol{\nu} = \frac{\mathbf{1}}{\mathbf{R}}$.

NS_{irr}: $\dot{u}_\alpha = -(\vec{u}\cdot\boldsymbol{\partial})u_\alpha - \partial_\alpha p + \frac{1}{R}\Delta u_\alpha + F_\alpha, \qquad \partial_\alpha u_\alpha = 0$

Velocity: $\vec{u}(x) = \sum_{\vec{k}\neq\vec{0}} u_{\mathbf{k}} \frac{i\mathbf{k}^\perp}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \overline{u}_{\mathbf{k}} = u_{-\mathbf{k}}$ (NS-2D)

$NS_{2,irr}$: $\dot{u}_{\mathbf{k}} = \sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}} \frac{(\mathbf{k}_1^\perp\cdot\mathbf{k}_2)(\mathbf{k}_2^2-\mathbf{k}_1^2)}{2|\mathbf{k}_1||\mathbf{k}_2||\mathbf{k}|} u_{\mathbf{k}_1}u_{\mathbf{k}_2} - \nu\mathbf{k}^2 u_{\mathbf{k}} + f_{\mathbf{k}}$

Immagine to truncate eq. supposing $|k_j| \le V$. Il taglio 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 $IS_t = S_{-t}I$, $\Rightarrow$: irreversibility.

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

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

$E_R = \int_{M_V} \mu_R^{i,V}(du)||u||_2^2, \qquad En_R = \int_{M_V} \mu_R^{i,V}(du)||\mathbf{k}u||_2^2$

Consider new equation, NS_{rev}:

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

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

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

New eq. is reversible: $IS_t u = S_{-t} Iu$ (as α is odd).
α is "a reversible viscosity"; (if $D = 3$ α 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 $\mathcal{E}^{r,V}$ on M_V: $\mu_{En}^{r,V}$ parameterized by the constant value of **enstrophy** $En = \sum_{\mathbf{k}} |\mathbf{k}|^2 |u_{\mathbf{k}}|^2$.

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

A first conjecture at small ν concerns the observables of large scale $O \in \mathcal{C}^\omega(M_V)$, *i.e.* analytic functions on the periodic container *i.e.* functions O on M_V with Fourier's transform *decaying exponentially* (uniformly in V)

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

$$\mu_R^{i,V}(\mathcal{D}) = En, \qquad \text{or} \qquad \mu_{En}^{r,V}(\alpha) = \frac{1}{R}$$

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

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

here $\mathcal{D}(\mathbf{u}) = \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2$. Hence time averaging

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

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

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

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

$$\mu_R^{i,V}(O) = \mu_{En}^{r,V}(O)(1 + o(1/R)) \qquad \textbf{se} \qquad \mu_R^{i,V}(\mathcal{D}) = En$$

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 ($V < \infty$), [1],
(2) NS with Ekman friction ($-\nu\vec{u}$ 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.

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 $\mathbf{u_k}$ 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 $V \to \infty$ from distributions $\mu_R^{i,V}, \mu_{En}^{r,V}$:

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

provided $\mu_R^{i,V}(\mathcal{D}) = En$, which therefore implies $R\mu^{r,V}(\alpha) \xrightarrow[V\to\infty]{} = 1$.

Analogy with equilibrium statistical mechanics is manifest

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

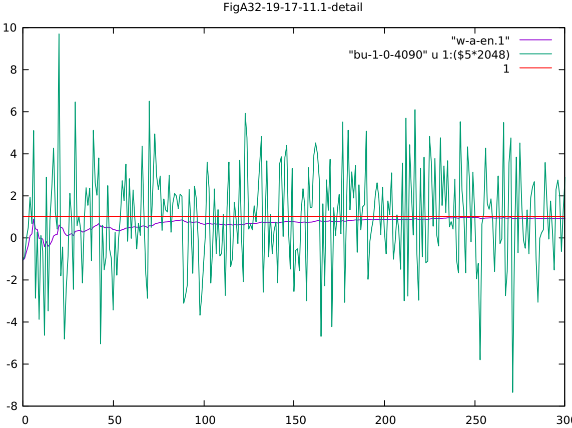
(b) K restricts to local observables

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

Conjectures → suggest several measurements to reveal the reversibility hidden in the NS_{irr}.

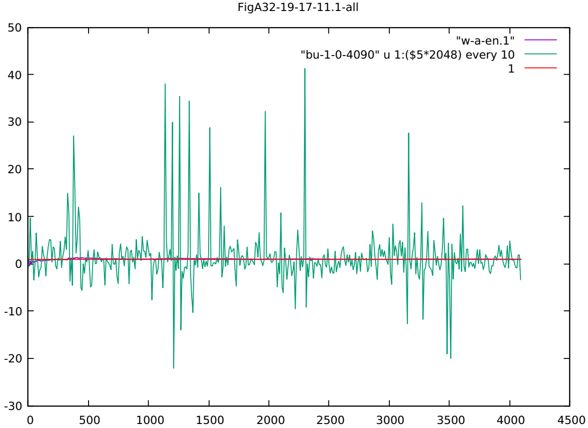
But it will be useful to pause to illustrate a few prelimnary simulations and checks.

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 would be perfectly capable to perform detailed checks in rapid time.



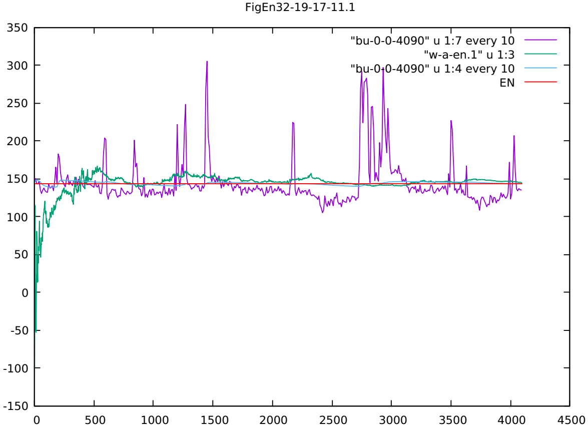
FigA32-19-17-11.1-detail

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. Evolution is NS_{rev}, **R=2048**, 224 modes, Lyap.$\simeq$ 2, x-unità 2^{19}



FigA32-19-17-11.1-all

Fig.1: AS previous fig. but time 10 times: data reported "every 10", **or** black.



FigEN32-19-17-11.1

Fig.2: **Running** average of the work $R\sum_{\mathbf{k}} F_{-\mathbf{k}} u_{\mathbf{k}}|$ (**Green**) in NS_{rev}; amd **convergence** to averages enstrophy $\sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$ (**red** straight line in NS_{rev},
green 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**.

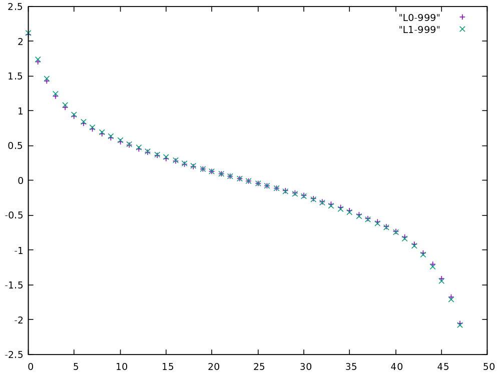


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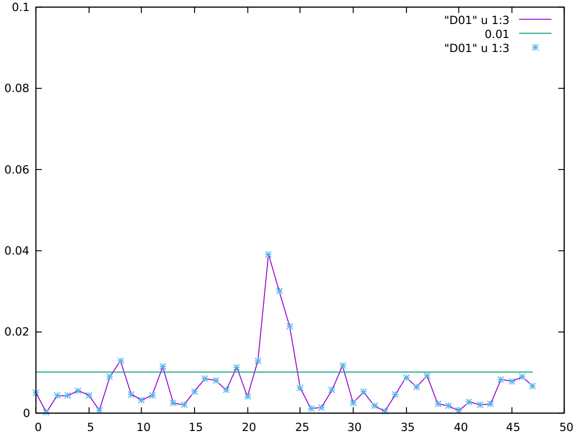
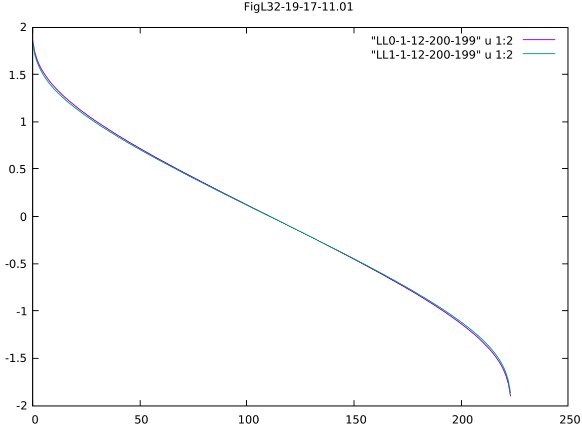
Fig.3: Spectrum (**local**) Lyapunov V=48 modes reversible & irreversible; **R=2048**.



FigDiff16-30-15-13-11.01-15

Fig.4: **Relative Difference** of (local) Lyap. exponents in Fig. preced. R=2048, 48 modes. Level line marks 1%.



FigL32-19-17-11.01

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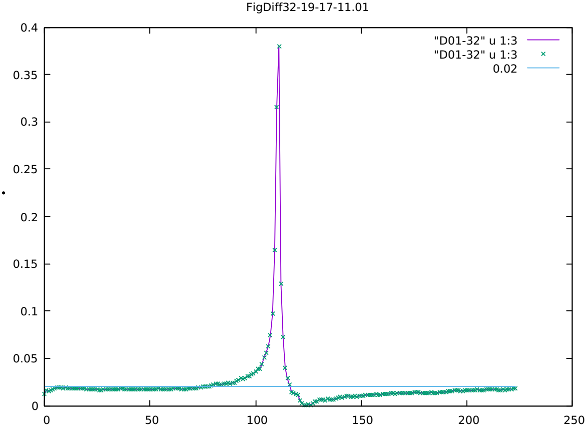
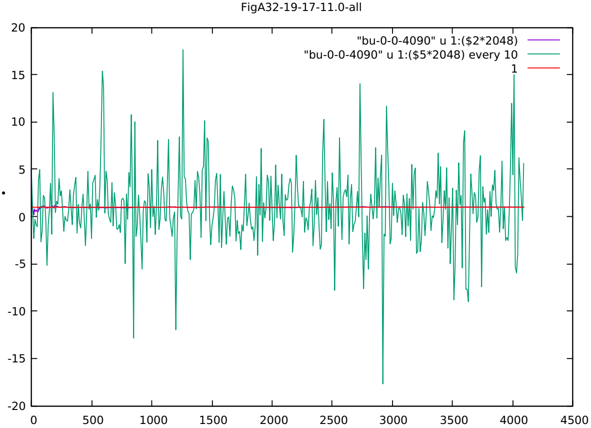
Fig.5: More Lyapunov spectrume in 15×15 modes (i.e. for NS2D rever. & irrev. $R = 2048$, 240 modes on 2^{13} steps. Spectra evalued every 2^{19} integr. steps. (and averaged over 200 samples).



FigDiff32-19-17-11.01

Fig.6: **Relative difference** of the (local) Lyapunov exp. of the preceding fig. 240 modes. The line is the 2% **level**.

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



FigA32-19-17-11.0-all

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):
(1) **Check** the "Fluctuation Relation" in the **irreversible** evollution: 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:

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

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.

Problema: se $\mathcal{A} \subset M_V$ e $\mathcal{A}$ ha dimensione inferiore, la simmetria di inv. temp. I è non applicabile perché $I\mathcal{A} \neq \mathcal{A}$. Questo certo avviene se V diventa abbastanza grande, [14, 15].

Supponiamo tuttavia che esista una simmetria P fra $\mathcal{A}$ e $I\mathcal{A}$ che commuta con l'evol. S_t: $PS_t = S_tP$. Allora $P \circ I : \mathcal{A} \to \mathcal{A}$ diventa una simmetria inversione tempo del moto su $\mathcal{A}$. E esistono condizioni geometriche che in casi speciali assicurano l'esistenza di P ("Assioma C", [16]).

Anche supponendo esistenza di P, ancora **non** si può applicare FR perché alla meglio riguarderebbe la $\sigma_{\mathcal{A}}(\mathbf{u})$ e non la $\sigma(\mathbf{u})$, ossia la contrazione della superficie di $\mathcal{A}$ e non di M_V.

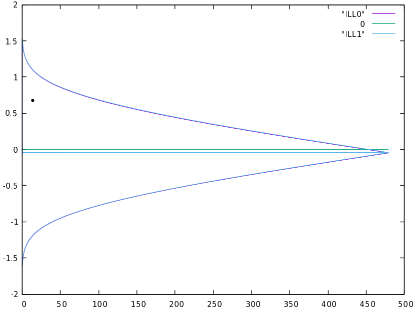
Però la $\sigma(\mathbf{u})$ riceve contributi dall'avvicinamento esponenziale a $\mathcal{A}$: che ovviamente non contribuiscono alla $\sigma_{\mathcal{A}}$. Ma come riconoscere tali contributi?

Aiuto da "regola di accoppiamento"

Spesso gli esponenti (locali e anche globali) si presentano in coppie con media quasi costante o disposta su una curva regolare.

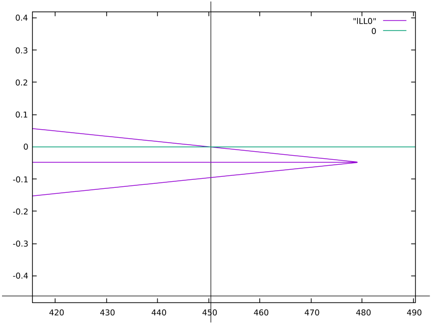
In molti sistemi le coppie hanno media esattamente costante (o comunque relativamente piccola a confronto agli elementi delle coppie).

Un'idea la si ottiene dagli esponenti locali (autovalori della parte simmetrica della linearizzazione del flusso (*i.e.* dalla matrice Jacobiana)).
Ad esempio in NS si può trovare:



FIGll-64-19-17-11

Fig.7: $R = 2048$, **960modi**, esponenti **locali** ordinati a decrescere λ_k, $0 \leq k < d/2$, a crescere $\lambda_{d-k}, 0 \leq k < d/2$ e le linee $\frac{1}{2}(\lambda_k + \lambda_{d-1-k})$ e la linea $\equiv 0$. Caso reversibile e irreversibile sovrapposti e apparente regola di accoppiamento.



FIGll-detail64-19-17-11

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Fig.8: Dettaglio Fig.7 mostra gli esp. NS_{irr} (solo) e la linea $\equiv 0$ e illustra la "perdita di dimensione" di $\frac{450}{490}$. See Ruelle: [14, Eq.(1.7)]. $R = 2048$, 960 modes.

Le figure presentano le caratteristiche:

(a) gli esp. revers. e irrrev. sono anche qui molto vicini: **non segue** dalla cong. (gli esp. non sono osserv. locali) $\rightarrow$ suggerisce: equivalenza per più vasta classe di osserv.

(b) Si è proposto che la superf. attraente $\mathcal{A}$ ha dimensione uguale doppio del numero di exponenti di Lyap. ≥ 0: se accoppiamento allora è 2 volte il num. di coppie ai segno $\pm$.

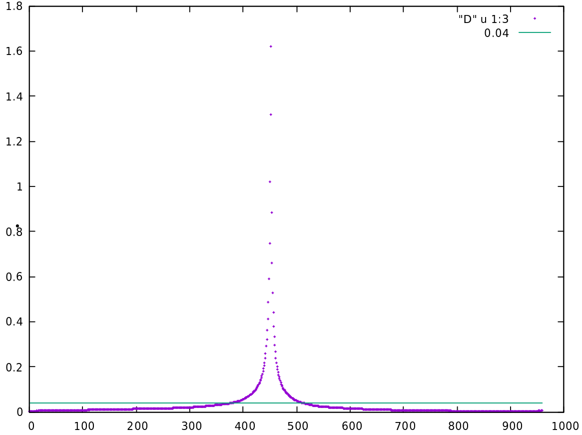
Implicazione: la $\sigma_{\mathcal{A}}(\mathbf{u})$ su $\mathcal{A}$ è proporzionale alla totale $\sigma(\mathbf{u})$

$$\sigma_{\mathcal{A}}(\mathbf{u}) = \boldsymbol{\varphi}\sigma(\mathbf{u}) = (1 - \frac{\sum_{opposite\ pairs}(\lambda_j + \lambda_j^*)}{\sum_{all\ pairs}(\lambda_j + \tau_j^*)})\sigma(\mathbf{u})$$

Idea: le coppie negative corrispondono agli exp. relativi alla attrazione ad $\mathcal{A}$: quindi non contano per il calcolo di $\sigma_{\mathcal{A}}$. Allora FR varrà, per l'I.C., ma con pendenza $\boldsymbol{\varphi} < 1$:

$$\tau p \boldsymbol{\varphi} \sigma, \quad \text{invece che} \quad \tau p \sigma : \quad \text{in fig. } \boldsymbol{\varphi} = \frac{\mathbf{450}}{\mathbf{490}}$$

Se vero: sarà controllo di reversibilità in NS_{irr}.



FIGdiff64-19-17-11

Fig.9: Differenza relativa $\frac{|\lambda_k^{rev}-\lambda_k^{irr}|}{\max(|\lambda_k^{rev}|,|\lambda_k^{irr}|)}$ fra esp. loc. reversibili e irreversibili in Fig.7. La linea è il livello 4% **level**.

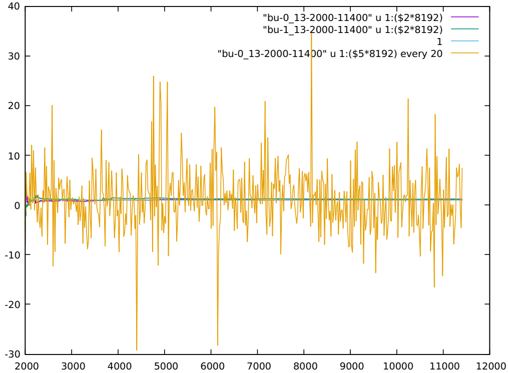
Controlli più elaborati in corso:

(a) momentidi osserv. di grande scala rev & irrev

(b) esponenti di Lyap. locali di altre matrici, invece che dello Jacobiano.

(c) controllo della relazione di fluttuazione, specie nel caso irrevers., che le fig. preced. mostrano essere acessibile già can 960 modi e $R = 2048$: $\Rightarrow$ FR con pendenza $\varphi < 1$ (Axiom C ?), [12, 11].

(d) altri R e N: un esempio interessante è la Fig.10 con R ben più grande dei casi precedenti:



FigA.0-13-2000-11400-13

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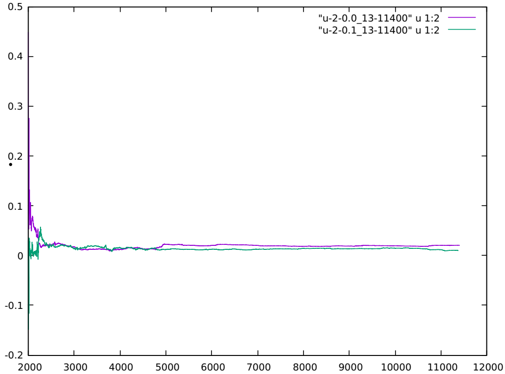
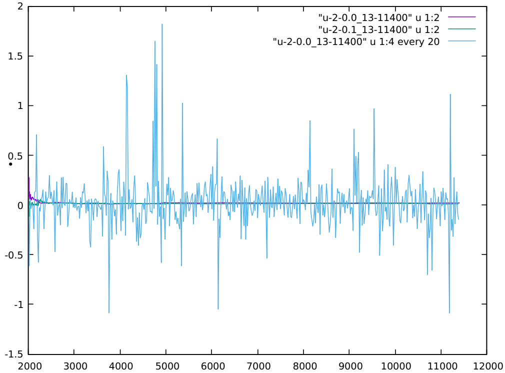
Fig.10: Higher $R = 8192$, 224 modes: running averages of $R\alpha(u)$ for NS_{irr} & NS_{rev}, (predicted 1) and fluctuations for the NS_{irr}. Time recorded every $4\lambda_{max}^{-1}$.

Esempio di momenti di osserv. locali :



Figu20-0/1-19-17-13

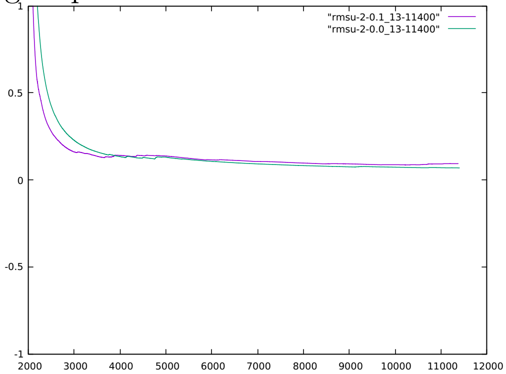
Fig.11: Medie correnti rev/irr di $|u_{20}|^2$, $R = 8192$, 224 modes.



Figu20-0/1-19-17-13

Fig.12: Stesse medie correnti rev/irr di $|u_{20}|^2$, con $R = 8192$, e anche le fluttuazioni (nel solo caso irr.), 224 modi.

Infine la rms della media rispetto alle fluttuazioni della Fig.12 precedente



FIGrmsu20-0/1-19-17-13

Fig.13: RMS per $|u_{20}|^2$ rev/irr, $R = 8192$, 224 modes

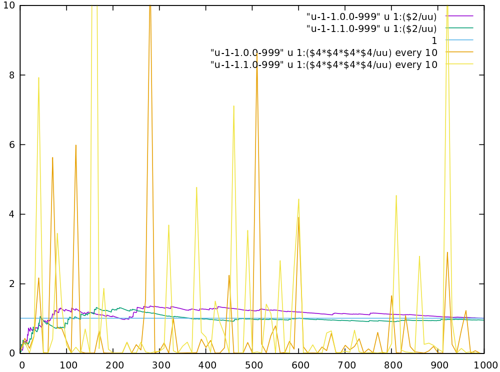


FIG16-u4-15-13-11.01

Fig.14: graph of $u^4_{1,1}/\langle\, u^4_{1,1}\,\rangle$, rev e irr con media corrente e flutt. $R = 2048$ e 48 modes. **controllo della cong.**

Infine è possibile una stima rigorosa del numero $\mathcal{N}$ di esp. di Lyap., locali e globali, necessari affinché ordinandoli a decrescere e sommandoli si trovi un valore < 0 (dimensione di KY)

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

in dimensione 2, mentre a dimensione 3 vale una stima simile ma espressa in termini di una norma diversa dalla enstrofia. La stimam di Ruelle se $d = 3$ e Lieb se $d = 2$, [17, 15], darebbe qui $\mathcal{N} \sim 2.10^4$: non controllabile nelle simulazioni presentate ma in linea di principio misurabile con i calcolatori e metodi di calcolo di NS già disponibili.

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].

Pur rinunciando a commentare l'affermazione sottolinei che la Meccanica Statistica, da Clausius, Boltzmann e Maxwell fu una semplice e sorprendente conseguenza della **"[wildly unphysical but well-understood]"** periodicità dei moti colletivi di 10^{19} molecole in un gas, [19].

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