Statistical ensembles out of equilibrium: turbulence

Equilibrium states $\Rightarrow \mathcal{N} = \rho V$ 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 $\rho(\mathbf{u})d\mathbf{u}$.

If 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}_{β}^{V} . 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 EH unifies equilibrium and nonequilibrium and assumes that generically chaotic systems are such in the precise sense of Axiom A implies also in nonequilibrium \Rightarrow unique statistics for the stationary states.

Axiom A can be simplified (Cohen & G) replacing it with "generically" chaotic motions evolve towards a smooth attracting surface over which motion is chaotic in the sense of Anosov (stronger than Axiom A): Chaotic hypothesis or CH.

Hence is 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.

Any theory of large (macrosc.) systems ⇒ requires
(1) Regularization of equations (via a "cut off")
(2) Restriction on observables ("local observables")

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

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.

L'Aquila, November 28 2019

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 on the paradigmatic case of periodic NS fluid, [1, 2].

L'Aquila, November 28 2019

(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 $\nu = \frac{1}{R}$

$$\begin{split} &NS_{irr}: \ \dot{u}_{\alpha} = -(\mathbf{u} \cdot \boldsymbol{\partial}) u_{\alpha} - \partial_{\alpha} p + \frac{1}{R} \Delta \mathbf{u}_{\alpha} + F_{\alpha}, \qquad \partial_{\alpha} u_{\alpha} = 0 \\ &\text{Velocity:} \ \mathbf{u}(x) = \sum_{\mathbf{k} \neq \mathbf{0}} u_{\mathbf{k}} \frac{i\mathbf{k}^{\perp}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \overline{u}_{\mathbf{k}} = u_{-\mathbf{k}} \quad (\text{NS-2D}) \\ &NS_{2,irr}: \ \dot{u}_{\mathbf{k}} = -\sum_{\mathbf{k}_{1}+\mathbf{k}_{2}=\mathbf{k}} \frac{(\mathbf{k}_{1}^{\perp}\cdot\mathbf{k}_{2})(\mathbf{k}_{2}^{2}-\mathbf{k}_{1}^{2})}{2|\mathbf{k}_{1}||\mathbf{k}_{2}||\mathbf{k}|} u_{\mathbf{k}_{1}} u_{\mathbf{k}_{2}} - \nu \mathbf{k}^{2} u_{\mathbf{k}} + f_{\mathbf{k}} \\ &\text{``Regularize eq.'': waves } |\mathbf{k}_{j}| \leq N. \text{ At } UV\text{-Cut-off }, N. \end{split}$$

Remark: $Iu_{\alpha} = -u_{\alpha}$ implies solutions $t \to S_t^{irr} \mathbf{u}$ s.t. $IS_t^{irr} \neq S_{-t}^{irr}I \implies \text{irreversibility}$ 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 $\mathcal{E}^{irr,N}$: This is 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.*:

 $E_R = \int_{M_N} \mu_R^{irr,N}(du) ||u||_2^2, \qquad En_R = \int_{M_N} \mu_R^{irr,N}(du) ||\mathbf{k}u||_2^2$ Are there other ensembles whose elements can be put in 1-1 correspondence with the ones in $\mathcal{E}^{irr,N}$ and give same average values to "local obsevables"? Consider new equation, NS_{rev} (with cut-off N):

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

with α 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 ~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 **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 same as $N \to \infty$ for

 $\mu_R^{irr,N} \in \mathcal{E}^{irr,N} \text{ and } \mu_{En}^{rev,N} \in \mathcal{E}^{rev,N}$

provided, $\mathcal{D}(\mathbf{u}) \stackrel{def}{=} \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2$ is s.t. $\mu_R^{irr,N}(\mathcal{D}) = En, \quad \text{or} \quad \mu_{En}^{rev,N}(\alpha) = \frac{1}{R} = \nu$

L'Aquila, November 28 2019

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.

Remark that W is a local observable

L'Aquila, November 28 2019

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.

L'Aquila, November 28 2019

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:

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

L'Aquila, November 28 2019



Fig.1 (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} , **R=2048**, 224 modes, Lyap. $\simeq 2$, x-unit = 2¹⁹



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

L'Aquila, November 28 2019



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**.

Unexpected



Fig.3: Fluct. max.-min. showing the N = 3968 NS_{rev} -exponents. Central lines rev-irr. superposed averaged over 800 samples with remarkable coincidence of NS_{rev} with the NS_{irr} exponents. Strong fluct. between max-min variations (upper and lower lines)

L'Aquila, November 28 2019

The following Fig.4 (similar to Fig.1 but w. NS_{irr}):



The figure suggests (from the theory of Anosov systems): **Check** the "Fluctuation Relation" in the **reversible** evolutions: 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:

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

Replacing reversible evolution with irreversible but studying the reversible divergence becomes a "reversibility test on the irreversible flow"!

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, [7, 8].

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} .

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 for both problems could come from "pairing property" 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 Jacobian matrix).

For instance NS seems to enjoy a pairing rule: the following figure illustrates it (at strong regularization and the large Reynolds number); looks close to exact (at graph scale!).

Pairing in NS cannot stay at all regularizations: the above should be considered due to the small N. However it has been proposed that the apparent "pairing line" becomes at large N a "pairing curve" (as apparently so at small R).



Fig.5: 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 $\varphi \simeq \frac{1500}{1980}$.

In Anosov reversible systems the number of positive exp. = number of negative: hence proposal, [9, p.445], [10],

"attracting surface \mathcal{A} dimension = twice the number of positive exponents" and

if pairing: 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

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

(for 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 exponents associated with attraction to \mathcal{A} : hence irrelevant in computating $\sigma_{\mathcal{A}}$. Assuming existence of P, hence time-reversal on attractor, and pairing + CH \Rightarrow FR but slope $\varphi < 1$: $\tau p \varphi \sigma$, rather than $\tau p \sigma$: in fig. $\varphi \simeq \frac{1550}{2490}$ If true: this will be a "check of reversibility" in NS_{irr} . More elaborate checks are being attempted: [6, 11] +(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?), [9, 12]. (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.6: Running averages in NS_{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



their rev. fluctuations, for R = 2048, 960 modes.

Concluding the simulation



Fig.8: Illustration of the conjecture on a 3968 modes NS: the running averages 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:

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

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, [13, 8]).

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, [14, p.344-347] and [2, app.A].

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