Reversibility, Navier-Stokes equations and nonequilibrium ensembles

Recent progress has been (partly) 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 = fundamental symmetry while friction = 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 leads to 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 $\mathcal{F}^C$" 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 $\mathbf{u}(\mathbf{x})=\sum_{\mathbf{k}}\mathbf{u}_{\mathbf{k}}e^{-2\pi\, i\,\mathbf{k}\cdot\mathbf{x}}, \mathbf{u}_{\mathbf{k}}=\overline{\mathbf{u}}_{-\mathbf{k}}$:

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

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

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

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*, and 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 $|\mathbf{k}|<N$ playing the role, as $N\to\infty$, of the thermodynamic limit.

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

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

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

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

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

(1): Vary $\nu \equiv \frac{1}{R}$ and let $\boldsymbol{\mu}_R^C$ stationary distrib. for **(*)** (I-NS). Define, for each R:

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

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

(2): Next consider the new equation (R-NS) **(**)**: 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.; define for each $\mathcal{E}$:

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

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

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

$$i)\ \mathcal{E} = \boldsymbol{\mu}_{R}^{C}(\mathcal{D}(\cdot))$$
$$ii)\ \nu = \boldsymbol{\mu}_{\mathcal{E}}^{M}(\alpha(\cdot))$$

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" $\boldsymbol{\mu}_{\beta}^{C}$ = "microcanonical" $\boldsymbol{\mu}_{\mathcal{E}}^{M}$.

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

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

A precise form of the conjecture could be
(1) define the distributions $\mu^C_R, \mu^M_{\mathcal{E}}$ as the limits

$$\mu^C_R = \lim_{N\to\infty} \mu^C_{R,N}, \qquad \mu^M_R = \lim_{N\to\infty} \mu^M_{\mathcal{E},N}$$

with $\mu^C_{R,N}, \mu^M_{\mathcal{E},N}$ defined as the stationary distributions for NS eq. truncated by setting $u_{\mathbf{k}} = 0$ for $|k_i| > N, i = 1, 2$
(2) *Given K-local observable $F, ||F|| < 1$ the averages of F with respect to a pair of equivalent distributions $\mu^C_{R,N}, \mu^M_{\mathcal{E},N}$ are related by*

$$\mu^C_{R,N}(F) = \mu^M_{\mathcal{E},N}(F)(1 + o_K(N, R))$$

with $o_K(N, R) \xrightarrow[N\to\infty]{} 0, \forall R,$ and $o_K(N, R) \xrightarrow[R\to\infty]{} 0, \forall N$

It should be stressed that the entire analysis does not depend on (non existent if $D = 3$) uniqueness results on NS and can be *verbatim* applied to the $3D$ case (defining $\alpha(\mathbf{u})$ do that $\mathcal{D}(\mathbf{u})$ is a constant of motion).

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 $\sigma_N(\mathbf{u}) \stackrel{def}{=} \mathrm{div}\Big(\alpha(\mathbf{u})\Delta\mathbf{u}\Big)$ averaged over a time τ

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

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, (see [9, 20]).

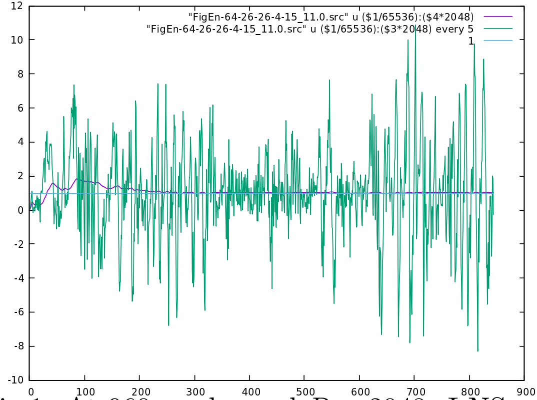
$$\frac{Prob_\tau(p)}{Prob_\tau(-p)} = e^{\tau\langle\,\sigma_N\,\rangle p + o(\tau)}, \qquad \tau \to \infty \qquad\qquad \textbf{(FR)}$$

Equivalence applied to the reversible viscosity ensemble $\mathcal{F}_{\mathcal{E}}^{M}$ and if extended to the observable $\sigma_N(\mathbf{u})$ would imply that $\sigma_N(\mathbf{u})$ fluctuates according to FR in the corresponding $\mathcal{F}_R^C$.

The equivalence condition $\mu_{\mathcal{E}}^{M}(\alpha(\mathbf{u})) = 1/R$ should come together **(?)** with a close relation between averages

$$\mu_R^C(\alpha(\mathbf{u})) \simeq 1/R$$

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).



FigA2-64-26-26-4-15-11.0

Fig.1: At 960 modes and $R = 2048$: I-NS evolution of

$$R\alpha(\mathbf{u}) = R\frac{\sum |\mathbf{k}|^2 \mathbf{g_k}\overline{\mathbf{u}}_\mathbf{k}}{\sum |\mathbf{k}|^4 |\mathbf{u_k}|^2} \qquad \text{“reversible viscosity”}$$

Equivalence $\rightarrow$ time average of α should be $\mathbf{\frac{1}{R}}$. Represents the fluctuating values of α at intervals of $5 \cdot 2^{15}$ integration steps of size 2^{-15}; the middle line is the running average of α and it converges to $\mathbf{\frac{1}{R}}$ (horiz. line).

The graph gives the values only every $5 \cdot 2^{15}$ integration steps (it would be too dense at every 2^{15}).

The experiments are carried using a truncated version of the I-NS eq. with cut-off at $|k_i| < N$: the conjecture requires the limit $N \to \infty$, or $R \to \infty$: hence it can be tested only by trying to compare stability of results with increasing N or R and (so far the max N reached is $N = 15$, but work is in progress).

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 need further confirmation).

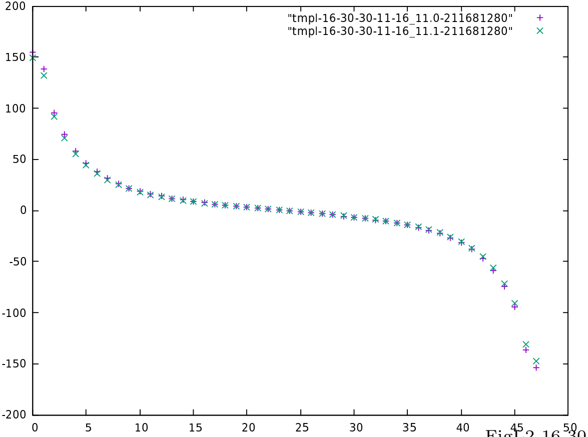


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Fig.2: T-Local Lyapunov spectrum: 48 modes (7×7) of NS2D: $(+)=$ viscous, $(\times)=$ reversible and $R = 2048$. Integration step 2^{-16}, $T = 2048$, integration steps 2^{30}.

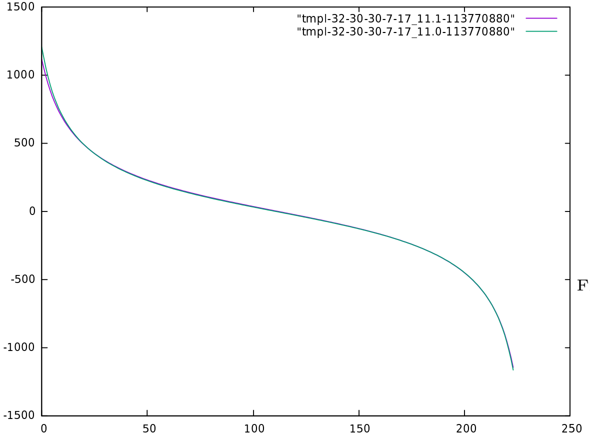

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Fig.3: Graph of the Lyapunov spectra in a 15×15 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1) with (the 224 points) interpolated by lines, $R = 2048$. 914 exponents evaluated every 2^{17} integration steps.

It is interesting to look at the fluctuations of $\mathcal{D}(\mathbf{u})$ in the I-NS **while** the Lyapunov exponents of the previous Fig.3 are measured:

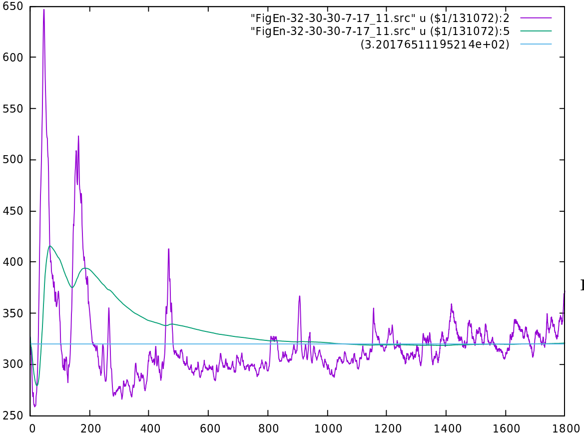

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Fig.4: enstrophy history (every 2^{17} integration steps), running average and precomputed average of $\mathcal{E}$.

The evolution of the reversible viscosity $R\alpha(\mathbf{u})$ measured in the I-NS (*i.e.* irreversible) evolution while the same local exponents in Fig.3 are computed is illustrated as:

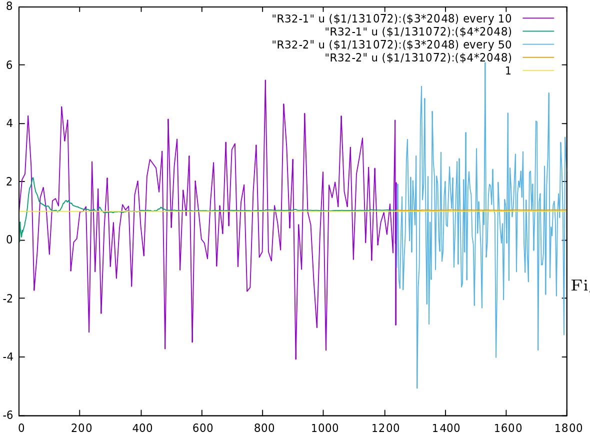

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Fig.5: I-NS evolution of the reversible viscosity $R\alpha(\mathbf{u})$ in the same time interval as Fig.4 (and in the computation of Fig.3).

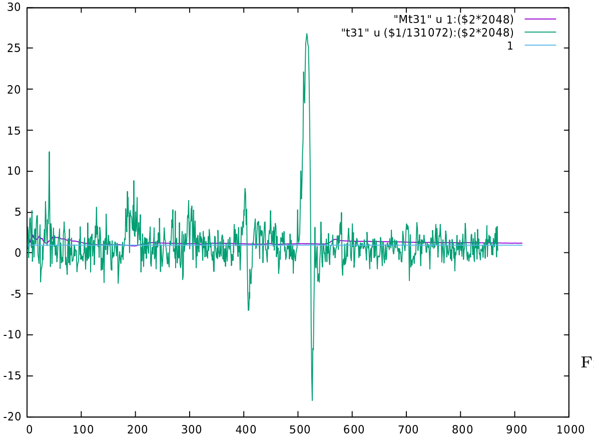

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Fig.6: R-NS evolution of $R\alpha(\mathbf{u})$: reversible viscosity, history, running average, and level 1.

The relative values of the local L. exponents is indistinguishable in the graphs above; following two figures draw the relative difference between the local exponents represented, respectively, in Fig.2 and Fig.3 (in percent):

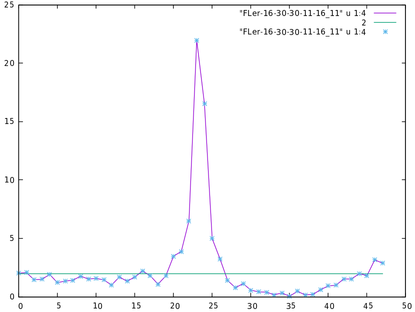

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Fig.7: relative difference of corresponding exponents in Fig.2.

The agreement between the corresponding Lyapunov exponents is below 2% except for the (seven) exponents close to 0. It is below 5% except of four exponents.

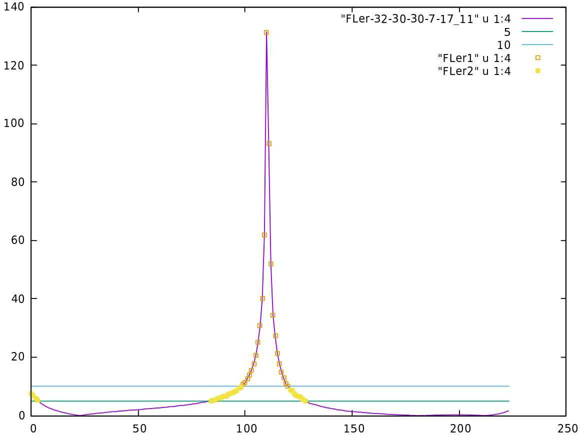

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Fig.8: relative difference of corresponding exps. in Fig.3.

The relative sizes are defined as 100 times the absolute value of the difference of correspoanding exponents divided by the maximum value of the two.

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 suggested 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).

(2) The observable $\mathcal{D}(\vec{u})$ should not play a special role: it could be replaced by other "global" oservables, *e.g.* 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** (*i.e.* $\mathbf{u}_{\mathbf{k}}$ with $2^n < |\mathbf{k}| \le 2^{n+1}$ $\to$ " n-th shell") was fixed to the OK41-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 or N 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) A new ensemble equivalent to $\mathcal{F}^C, \mathcal{F}^M$ could be constructed replacing the viscosity with a white Gaussian process, with average satisfying the fluctuation relation **(?)**

(b) Are the fluctuations of the reversible friction observed in the irreversible evolution a stochastic process obeying a fluctuation relation (see Fig. above)? a further way to reveal reversibility in the irreversible evolution ?

Quoted references

[1] D. J. Evans and G. P. Morriss.
Statistical Mechanics of Nonequilibrium Fluids.
Academic Press, New-York, 1990.

[2] S. Nosé.
A unified formulation of the constant temperature molecular dynamics methods.
Journal of Chemical Physics, 81:511–519, 1984.

[3] W. Hoover.
Canonical equilibrium phase-space distributions.
Physical Review A, 31:1695–1697, 1985.

[4] Z.S. She and E. Jackson.
Constrained Euler system for Navier-Stokes turbulence.
Physical Review Letters, 70:1255–1258, 1993.

[5] J.C. Maxwell.
Illustrations of the dynamical theory of gases.
In: The Scientific Papers of J.C. Maxwell, Cambridge University Press, Ed. W.D. Niven, Vol.1, pages 377–409, 1860.

[6] J.C. Maxwell.
On the dynamical theory of gases.
In: The Scientific Papers of J.C. Maxwell, Cambridge University Press, Ed. W.D. Niven, Vol.2, pages 26–78, 1866.

[7] L. Boltzmann.
Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen.
Wiener Berichte, 63, (W.A.,#22):275–370, (316–402), 1872.

[8] G. Gallavotti.
Equivalence of dynamical ensembles and Navier Stokes equations.
Physics Letters A, 223:91–95, 1996.

[9] G. Gallavotti.
Dynamical ensembles equivalence in fluid mechanics.

Physica D, 105:163–184, 1997.

[10] D. Ruelle.
A remark on the equivalence of isokinetic and isoenergetic thermostats in the thermodynamic limit.
Journal of Statistical Physics, 100:757–763, 2000.

[11] D. Ruelle.
Turbulence, strange attractors and chaos.
World Scientific, New-York, 1995.

[12] Ya. G. Sinai.
Topics in ergodic theory, volume 44 of *Princeton Mathematical Series*.
Princeton University Press, 1994.

[13] G. Gallavotti.
Breakdown and regeneration of time reversal symmetry in nonequilibrium statistical mechanics.
Physica D, 112:250–257, 1998.

[14] D. Ruelle.
Measures describing a turbulent flow.
Annals of the New York Academy of Sciences, 357:1–9, 1980.

[15] G. Gallavotti and D. Cohen.
Dynamical ensembles in stationary states.
Journal of Statistical Physics, 80:931–970, 1995.

[16] G. Gallavotti.
Ergodicity: a historical perspective. equilibrium and nonequilibrium.
Eur. Phys. J. H., 41, online-first:1–80, 2016.

[17] G. Gallavotti.
Nonequilibrium and irreversibility.
Theoretical and Mathematical Physics. Springer-Verlag and http://ipparco.roma1.infn.it & arXiv 1311.6448, Heidelberg, 2014.

[18] D. Ruelle and F. Takens.

On the nature of turbulence.
Communications in Mathematical Physics, 20:167–192, 1971.

[19] G. Gallavotti and D. Cohen.
Dynamical ensembles in nonequilibrium statistical mechanics.
Physical Review Letters, 74:2694–2697, 1995.

[20] F. Bonetto and G. Gallavotti.
Reversibility, coarse graining and the chaoticity principle.
Communications in Mathematical Physics, 189:263–276, 1997.

[21] V. Franceschini, C. Tebaldi, and F. Zironi.
Fixed point limit behavior of N-mode truncated Navier-Stokes equations as N increases.
Journal of Statistical Physics, 35:387–397, 1984.

[22] G. Gallavotti, L. Rondoni, and E. Segre.
Lyapunov spectra and nonequilibrium ensembles equivalence in 2d fluid.
Physica D, 187:358–369, 2004.

[23] L. Rondoni and C. Mejia-Monasterio.
Fluctuations in nonequilibrium statistical mechanics: models, mathematical theory, physical mechanisms.
Nonlinearity, 20:R1–R37, 2007.

[24] L. Fang, J.T.W. Bos, L. Shao, and JP. Bertoglio.
Time reversibility of NavierStokes turbulence and its implication for subgrid scale models.
Journal of Turbulence, page 114, 2012.

Also: http://arxiv.org & http://ipparco.roma1.infn.it

Slides, edited, of the talk at the Rutgers seminar on 2 Nov 2017.