Reversibility, Irreversibility, Friction and nonequilibrium ensembles in N-S equations

Question: can the phenomenological notion of friction be represented in <u>alternative</u> ways?

Here is an attempt to answer yes by relating the problem to that of setting up a theory of statistical ensembles, and their equivalence, extending to stationary non-equilibria the ideas behind the canonical and microcanonical ensembles.

Idea: a fundamental symmetry like "time reversal" (or *PCT*) cannot be "spontaneouly broken"

Therefore even the stationary states of dissipative systems ought to be describable via time reversible equations.

Equilibrium ensembles theory provides key to proceed: it will be better to consider a paradigmatic example, the NS fluid in a periodic box, 2D. $R \equiv \frac{1}{\nu}$ be Reynolds number.

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

Although the 2D NS admit general smooth solution it is convenient to imagine NS equation as truncated at $|\mathbf{k}| \leq N$. The cut-off N will be fixed for a while.

The NS become 4N(N+1) ODE's on phase space M_N .

 $Iu_{\alpha} = -u_{\alpha}$ does not imply $IS_t \neq S_{-t}I$, \Rightarrow : these are irreversible equations.

Let u be an initial state: then $t \to S_t u$ evolves and generates a stationary state on M_N which, aside exceptions collected in a 0-volume in M_N , is supposed unique. Let $\mu_R(du)$ be its PDF. Stationary PDFs generalize equilibrium ones: thus collection \mathcal{E}^c of the $\mu_R(du)$ will be called an **ensemble of nonequil.** distrib. for NS_{irr} .

Hence average energy E_R , average dissipation En_R , Lyapunov spectra \mathcal{L}_R ..., will be defined, *e.g.*:

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

Consider the new equation, NS_{rev} :

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

with α s. that $En(u) = ||\mathbf{k}u||_2^2$ is exact constant of motion:

$$\alpha(u) = \frac{\sum_{\mathbf{k}} \mathbf{k}^2 Re(F_{-\mathbf{k}} u_{\mathbf{k}})}{\sum_{\mathbf{k}} \mathbf{k}^4 |u_{\mathbf{k}}|^2} \quad \text{if } D = 2$$

The new equation is reversible: $IS_t u = S_{-t}Iu$ (as α is odd).

So α is "reversible friction"; (if D = 3 slightly different)

This can be thought as a "thermostat" acting on the system and it should (?) have same effect as onstant friction.

The evolution with NS_{rev} generates a family of stationary distributions on phase space: μ_{En}^{mc} parameterized by the constant value of the dissipation $En = \sum_{\mathbf{k}} |\mathbf{k}|^2 |u_{\mathbf{k}}|^2$. Denote \mathcal{E}^{mc} such collection of stationary PDFs.

The $\alpha(u)$ in NS_{rev} will fluctuate strongly if the Reynolds number is large and it will "self-average" to a constant ν thus "homogenizing" the equation and turning it into the NS_{irr} with friction ν . A first more precise statement:

The averages of large scale observables will show the same statistical properties, as $R \to \infty$, in the NS_{irr} and in the NS_{rev} equations under the correspondence

 $\mu_R^c \longleftrightarrow \mu_{En}^{mc} \quad if \quad \mu_R^{mc}(En(u)) = En$

By large scale observables it is simply meant "observables depending on the Fourier's components $u_{\mathbf{k}}$ with $|\mathbf{k}| < K$ with some fixed K". And given K and such an observable it should be

$$\mu_R^c(O) = \mu_{En}^{mc}(O)(1 + o(1/R)) \quad \text{if}$$

$$\mu_{En}^{mc}(\alpha) = \frac{1}{\mathbf{R}} \quad \text{or} \quad \mu_{\mathbf{R}}^c(||\mathbf{ku}||^2) = \mathbf{En}$$

Recalls canon.-microcan. equivalence: $\nu = \frac{1}{R}$ plays the role of the canonical temperature (β) and En that of microcanonical energy.

Is the limit $R \to \infty$ the analogue of the thermodynamic limit?

Distinguish two cases. In case 1 model does not follow from fundamental microscopic dynamics: it is just a phenomen. descr. of a reversible system with friction added.

Examples,

- (1) (highly) truncated NS equations $(N < \infty)$, [1, 2]
- (2) NS with Ekman friction, [3, 4],
- (3) Lorenz96 model, [5],
- (4) Turbulence shell model, (GOY), [6]

where the equivalence is achieved only in the limit of infinite forcing.

Case 2 is that of the Navier Stokes equation: which can be derived from first principles. For instance in the NS_{irr} equation (derived by Maxwell from molecular motion, [7]) it is natural to think that there should be no condition for strong chaos.

The microscopic motion is always strongly chaotic and the chaotic condition should be always fulfilled even when **motion appears laminar**.

To pursue this suggestion consider the truncated $NS_{rev/irr}$ equations at momentum N: in dimension 2 or 3. Then The large scale observables, depending on the modes $|\mathbf{k}| < K$, have a the same statistics in corresponding PDFs in \mathcal{E}^c and \mathcal{E}^{mc} in the limit $N \to \infty$ for all R or En

The analogy with Equilibrium Statistical Mechanics becomes much clearer:

(a) The (necessary if D = 3) cut-off N plays the role of the finite volume container

(b) the large scale cut-off K restricts attention to the local observables

c) the Reynolds number R plays the role of inverse temperature β and the dissipation En the role of the microcanonical energy. Then

 $\lim_{N \to \infty} \mu_{En}^{mc}(O) = \lim_{N \to \infty} \mu_R^c(O)$

for O(u) depending on $u_{\mathbf{k}}$ with $|\mathbf{k}| < K$ and under the equivalence relation (*i.e.* $\mu_{En}^{mc}(\alpha) = \frac{1}{R}$): of course the larger K the larger N needs to be, just as in equilibrium Stat. Mech.

The above equivalence conjectures open the way to perform measurements on real fluids which reveal the "hidden" reversibility of the motions.

At this point it is convenient to pause and show a few results of simulations which begin to test the equivalence proposal.

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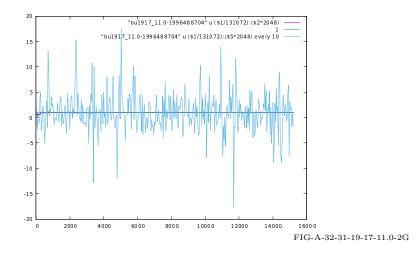


Fig.1: The running average of the reversible friction $R\alpha(u) \equiv R \frac{2Re(f_{-\mathbf{k}_0}u_{\mathbf{k}_0})\mathbf{k}_0^2}{\sum_{\mathbf{k}}\mathbf{k}^4|u_{\mathbf{k}}|^2}$, superposed to the conjectured value 1 and to the fluctuating values $R\alpha(u)$: Evolution NS_{irr} , **R=2048**

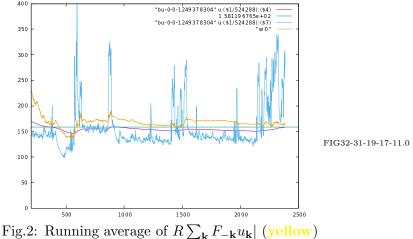


Fig.2: Running average of $R \sum_{\mathbf{k}} F_{-\mathbf{k}} u_{\mathbf{k}}|$ (yellow) converges to the average of $\sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$ (straight blue line) **Brown** line = running average of $\sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$ large fluctuations are those of $\sum_{\mathbf{k}}^2 |u_{\mathbf{k}}|^2$: Evolution NS_{irr} , $\mathbf{R}=2048$

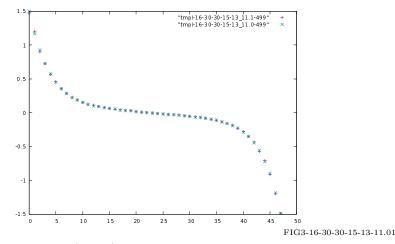


Fig.3: The (local) Lyapunov spectra for 48 modes truncation: reversible and irreversible. And almost pairing, alertbR=2048.

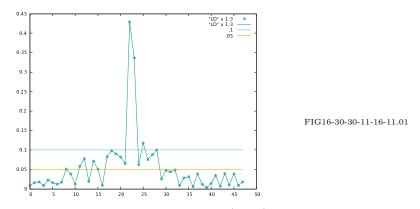


Fig.4: Relative difference betweeen (local) Lyapunov exponents. R=2048

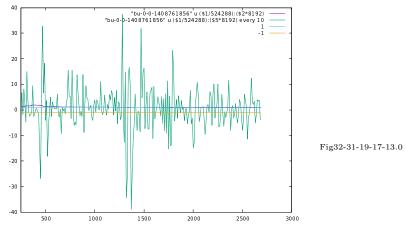


Fig.5: The running average of the reversible friction $R\alpha(u) \equiv R \frac{2Re(f_{-\mathbf{k}_0} u_{\mathbf{k}_0}) \mathbf{k}_0^2}{\sum_{\mathbf{k}} \mathbf{k}^4 |u_{\mathbf{k}}|^2}$, superposed to the conjectured value 1 and to the fluctuating values $R\alpha(u)$: Evolution NS_{irr} , levels ± 1 marked, **R=8192**.

The last fig. suggests:

(1) Test the Fluctuation relation in the linearized **irreversible** evolution of the Jacobian

$$\dot{\delta}_{\mathbf{k}} = \sum_{\theta=\pm 1,\mathbf{h}}^{*} g(\theta \,\mathbf{h},\mathbf{k}) u_{\mathbf{k}-\theta \,\mathbf{h}} \delta_{\mathbf{h}} - \frac{1}{R} \mathbf{k}^{2} \delta_{\mathbf{k}}$$
$$g(\mathbf{h},\mathbf{k}) = \frac{(\mathbf{k}^{\perp} \cdot \mathbf{h})(\mathbf{k}^{2} - 2\mathbf{k} \cdot \mathbf{h})}{|\mathbf{h}||\mathbf{k}||\mathbf{k}||\mathbf{h}|}$$

(from which the divergence $\sigma(u)$ can be computed).

(2) If FR is respected then a new ensemble \mathcal{E}^{st} can be introduced consisting in the stationary states for the 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 gaussian process uncorrelated in time but with average $\langle \nu \rangle = \frac{1}{R}$ and PDF respecting the FR which means with dispersion equal to the average

More elaborate tests are under way:

(a) moments of large scale observables rev & irrev (b) study the (local) Lyapunov exponents of other matrices: for instance instead of the Jacobian use the matrix obtained by replacing $g(\mathbf{h}, \mathbf{k})$ by

$$\gamma(\mathbf{h}, \mathbf{k}) = \frac{(\mathbf{k} \cdot \mathbf{h})(\mathbf{k}^2 - 2\mathbf{k} \cdot \mathbf{h})}{|\mathbf{h}||\mathbf{k}||\mathbf{k}||\mathbf{h}|}$$

This is much more unstable and the (local) L. exp. are easier to compute. Preliminary results are quite promising. as shown in the next figure:

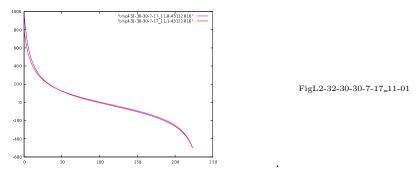


Fig.6: Lyapunov spectra in a 15×15 truncation for the NS2D with viscosity and reversible viscosity (captions ending respectively in 0 or 1) with (the 224 points) and matrix J^* , interpolated by lines, R = 2048. 914 are spectra evaluated, every 2^{17} integration steps (running average).

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