



Fluctuation Relation in a Shell Model of Turbulence



Collaborative Research Centre TRR 181
"Energy Transfers in Atmosphere and Ocean"

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(Sub-Project M4)

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Idea and Purpose of M4 — Entropy Production in Turbulence Parameterisations

The physically consistent representation of turbulence subgrid-scale processes in forced dissipative systems like atmosphere and ocean requires the handling of statistical nonequilibrium fluctuations. The statistics of these fluctuations — as a fingerprint of the chaotic dynamics — provide useful insights into the dynamical response behaviour of a system (transport coefficients) and can be described by the Fluctuation Theorem. The idea of M4 is the incorporation of this theorem to modify existing parameterisation schemes, focusing on a stochastic and counter-gradient parameterisation of momentum and heat fluxes which are related to energy dissipation and backscatter.

Fluctuation Theorem

- Result from statistical physics of **time-reversible** dynamical systems
- Different versions with constraint on probability distributions of fluctuations of non-equilibrium quantities (dissipation function, contraction rate, **entropy production**)
- Connection of microscopic reversibility and macroscopic irreversibility (**generalisation of the 2nd law of thermodynamics**)

Condition for Macroscopic Reversibility:

[Sevick EM, Prabhakar R, Williams SR, Searles DJ. 2008. *Annu. Rev. Phys. Chem.* 59:603-33] *

probability forward = probability backward

$$f(\Gamma_0, 0) \delta\Gamma_0 = f(\Gamma_t^*, 0) \delta\Gamma_t^*$$

$$\ln\left(\frac{f(\Gamma_0, 0) \delta\Gamma_0}{f(\Gamma_t^*, 0) \delta\Gamma_t^*}\right) \begin{cases} = 0 & \text{reversibility} \\ \neq 0 & \text{irreversibility} \end{cases}$$

Definition of an entropy-like quantity in nonequilibrium as a measure for macroscopic irreversibility

Dissipation Function $\Omega(\Gamma_t)$:
(generalised entropy production)

$$\bar{\Omega}_t = \frac{1}{t} \int_0^t \Omega(\Gamma_s) ds := \frac{1}{t} \ln\left(\frac{f(\Gamma_0, 0) \delta\Gamma_0}{f(\Gamma_t^*, 0) \delta\Gamma_t^*}\right) = \frac{1}{t} \ln\left(\frac{f(\Gamma_0, 0)/f(\Gamma_t^*, 0)}{\delta\Gamma_0/\delta\Gamma_t^*}\right)$$

Properties:

- Extensive phase variable (\propto system size)
- Odd under time-reversal

First case: dynamical system arbitrarily far from equilibrium

Transient Fluctuation Theorem (TFT)

[Evans DJ, Searles DJ. 2002. *Adv. Phys.* 51:1529-85]

$$p(\bar{\Omega}_t = A) / p(\bar{\Omega}_t = -A) = \exp(At)$$

with

$$\langle \bar{\Omega}_t \rangle \geq 0$$

- Equilibrium: $\langle \bar{\Omega}_t \rangle = 0$
- Close to equilibrium: $\bar{\Omega}_t$ related to entropy production σ (\propto flux \cdot force)
- Based on statistics of initial ensemble (**bundle of trajectories**)

Second case: dynamical system in steady state

Asymptotic version of TFT

Chaotic Hypothesis + Large Deviation
($p(X) \sim e^{tI(X)}$ ($t \rightarrow \infty$), $I(X) - I(-X) = X$)

Evans-Searles Steady-State Fluctuation Theorem

[Evans DJ, Searles DJ. 2002. *Adv. Phys.* 51:1529-85]

Transient state $\xrightarrow[\text{relaxation time } t_R]{}$ Steady state

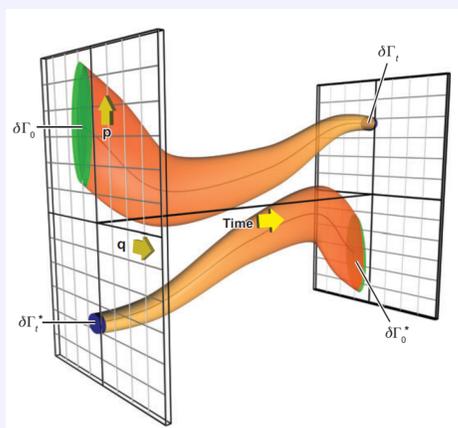
$$\lim_{t/t_R \rightarrow \infty} \frac{1}{t} \ln\left(\frac{p(\bar{\Omega}_{t,ss} = A)}{p(\bar{\Omega}_{t,ss} = -A)}\right) = A$$

Gallavotti-Cohen Fluctuation Theorem

[Gallavotti G, Cohen EGD. 1995. *J. Stat. Phys.* 80:931-70]

$$\lim_{t \rightarrow \infty} \frac{1}{t} \ln\left(\frac{p(\bar{\Lambda}_t = A)}{p(\bar{\Lambda}_t = -A)}\right) = A \quad (1)$$

- Thermostated systems: $\bar{\Lambda}_t$ related to entropy production
- Based on statistics of **single trajectory**



Bundle of trajectories (upper set) in phase space of a deterministic dissipative **time-reversible** system, $\dot{\Gamma} = F(\Gamma)$, starting within the volume $\delta\Gamma_0$ at point $\Gamma_0 = (q_0, p_0)$ with negative contraction rate $\Lambda = \nabla \cdot \dot{\Gamma}$. The probability for observing the system at a certain point Γ_t within the volume $\delta\Gamma_t$ at time t is given by $f(\Gamma_t, t) \delta\Gamma_t$. The distribution function $f(\Gamma_t, t)$ is determined by the Liouville equation $\partial_t f + \nabla \cdot (f \dot{\Gamma}) = 0$. The **Fluctuation Theorem** interrelates these probabilities with those for observing the system in a set containing the corresponding time-reversed trajectories (lower bundle with $\Gamma_t^* = (q_t, -p_t)$). [Ref. *, Fig. 1]

Shell Model of Turbulence

Atmosphere and ocean dynamics: **non-time-reversible** Navier Stokes equations

Studies of energy transfer mechanism in Fourier space

$$\frac{d}{dt} \hat{u}(\mathbf{k}, t) = \underbrace{\mathbf{N}(\mathbf{k}', \mathbf{k}'', t)}_{\text{triads interaction}} + \underbrace{\hat{\mathbf{f}}(\mathbf{k}, t)}_{\text{force term}} - \underbrace{\nu k^2 \hat{u}(\mathbf{k}, t)}_{\text{viscous term}}$$

Modeling of the nonlinear term:

- No geometry
- Reduction to N shells of wavenumbers
- Truncation of spectral modes
- Nearest-neighbour-interaction

Shells represented by complex velocities $\{u_n(t)\}$

GOY Shell Model (Gledzer 1973, Ohkitani & Yamada 1987)

[Aumaitre S, Fauve S, McNamara S, Poggi P. 2001. *Eur. Phys. J. B* 19: 449-60]

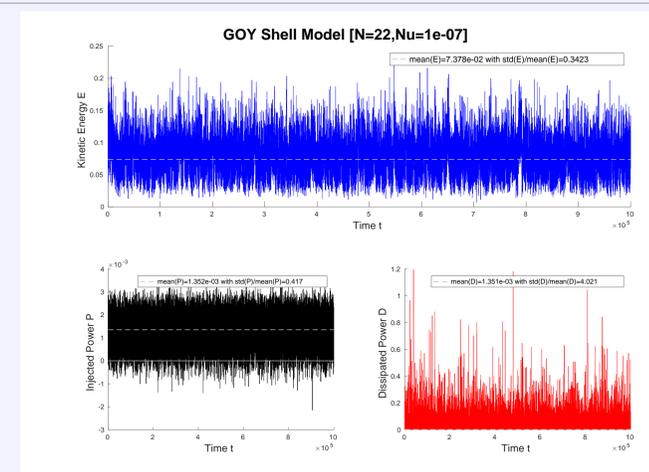
$$\frac{d}{dt} u_n = ik_n \underbrace{(u_{n+1}^* u_{n+2}^* - \frac{\alpha}{2} u_{n-1}^* u_{n+1}^* - \frac{1-\alpha}{4} u_{n-1}^* u_{n-2}^*)}_{\text{energy conserving}} + \underbrace{f \delta_{n,A}}_{\text{large scales}} - \underbrace{\nu k_n^2 u_n}_{\text{small scales}} \quad (n = 1, \dots, N)$$

Commonly used values for investigation of 3D turbulence:

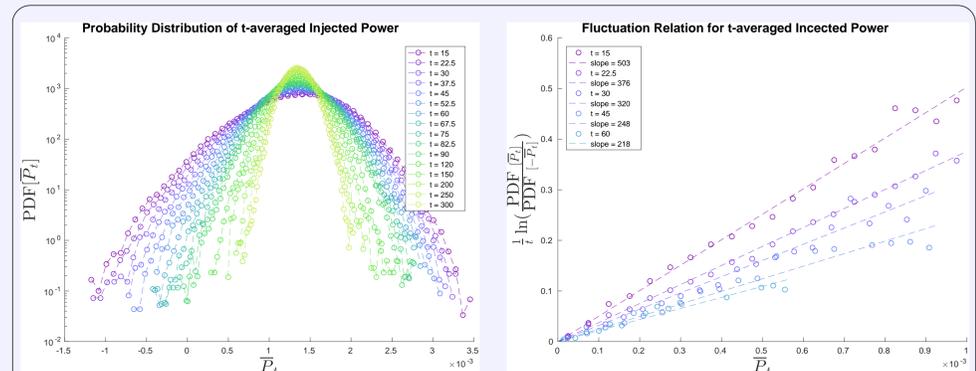
$$\alpha = \frac{1}{2}, k_n = 2^n k_0, k_0 = 2^{-4}, f = (5 + 5i) 10^{-3}$$

Energy balance equation: $\dot{E}(t) = P(t) - D(t)$

After passing the transient regime the system is in a statistically steady state with $\langle P \rangle = \langle D \rangle$. The contraction rate $\Lambda = -\nu \sum_{n=1}^N k_n^2$ is a non-fluctuating quantity. The validity of eq. (1) was tested for the injected Power with close-to-Gaussian distribution and a correlation time $t_c \approx 15$.



Statistics of time-averages $\bar{P}_t > t_c$



Results:

- Fluctuation relation (varying slope tending to a limit) shown in a shell model for statistics of averaged injected power \bar{P}_t (tested range: $-10^{-3} \leq \bar{P}_t \leq 10^{-3}$, $t \lesssim 70$)
- Distribution of normalised power $Y_t = \frac{\bar{P}_t}{P_\infty}$ described by $p(Y_t) \propto e^{-\beta(t) I(Y)}$ with scaling function $I(Y)$ and $\beta = At + B$, leading to **non-asymptotic** relation:

$$\ln\left(\frac{p(Y_t)}{p(-Y_t)}\right) = (At + B) Y_t$$

