MULTIPLICATIVE FLUCTUATION RELATIONS
in
SIMPLE MODELS of TURBULENT TRANSPORT

Krzysztof Gawedzki, Paris, IHP, Nov. 2007

Turbulent transport of particles or droplets is important for:

engineering, chemistry, environment studies, meteorology, astrophysics, cosmology

Simple modeling:

- **statistical description** of turbulent flows using synthetic random ensembles of velocities $\boldsymbol{v}_t(\boldsymbol{r})$
- **passive approximation** (no back-reaction of transported matter on the flow)
- **few collisions**

Aim: to discover and understand the origin of **robust features** rather than to provide a detailed quantitative description

Passive transport of particles:

- Lagrangian tracers with no inertia:

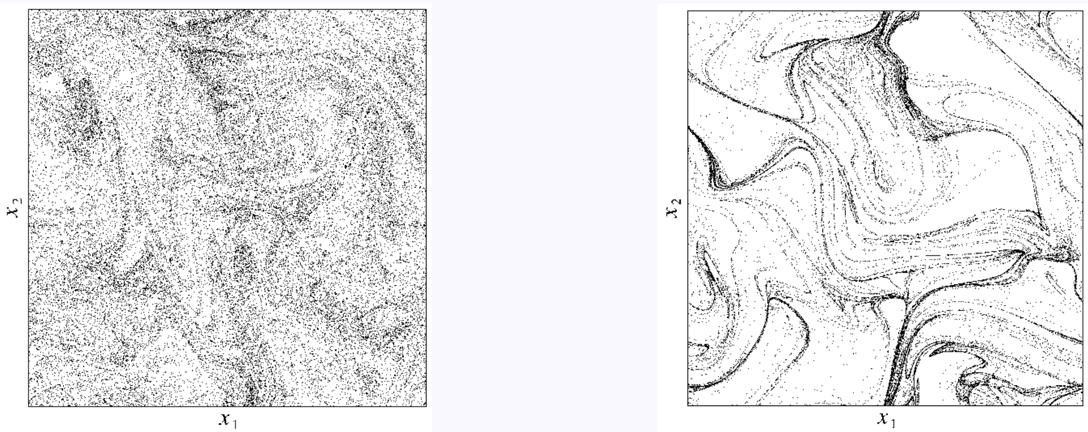
$$\dot{\boldsymbol{r}} = \boldsymbol{v}_t(\boldsymbol{r})$$

- particles with inertia:

friction force

$$\dot{\boldsymbol{r}} = \boldsymbol{v}, \qquad \dot{\boldsymbol{v}} = -\frac{1}{\tau}\big(\boldsymbol{v} - \boldsymbol{v}_t(\boldsymbol{r})\big)$$

Stokes time



from **J. Bec**, J. Fluid Mech. 528, 255-277 (2005)

Aim of this talk (based on joint work with Raphaël CHETRITE):

Search for a common ground between some recent ideas in **non-equilibrium statistical mechanics** and in **turbulence**

Particularly convenient place for such a search:

transport in **Kraichnan velocities**: Gaussian random ensemble of fields $\boldsymbol{v}_t(\boldsymbol{r})$ decorrelated in time widely used in last years to model turbulent phenomena

General mathematical setup:

dynamics defined by the **stochastic differential equation** (**SDE**)

$$\dot{x} \;=\; u_t(x) + v_t(x)$$

(with the Stratonovich convention), where $u_t(x)$ is a deterministic vector field and $v_t(x)$ is a random Gaussian field with zero mean and covariance

$$\big\langle v_t^i(x)\, v_s^j(y)\big\rangle \;=\; 2\,\delta(t-s)\, D^{ij}(x,y)$$

Solution x_t of the **SDE** $\dot{x} = u_t(x) + v_t(x)$ is a **Markov diffusion process** such that

$$\frac{d}{dt}\left\langle f(x_t)\right\rangle = \left\langle (L_t f)(x_t)\right\rangle$$

where the **generator** $L_t = \hat{u}_t^i \cdot \partial_i + \partial_i d_t^{ij} \partial_j$ with

$$\hat{u}_t^i(x) = u_t^i(x) - \partial_{y^j} D^{ij}(x,y)|_{y=x} \qquad \text{and} \qquad d_t^{ij}(x) = D^{ij}(x,x)$$

Common setup for:

- **deterministic dynamical systems**, e.g. chaotic
- **tracers** and **inertial particles** in the **Kraichnan velocities**
- in- and out-of-equilibrium **Langevin dynamics**
- **hydrodynamical limits** of stochastic lattice gases

(could be extended to non-Markovian processes)

- For **deterministic dynamical system**, the covariance

$$D_t^{ij}(x,y) \equiv 0$$

- For **Lagrangian tracers** in the **Kraichnan model**,

$$x \equiv \boldsymbol{r}\,, \qquad u_t(x) + v_t(x) = \boldsymbol{v}_t(\boldsymbol{r})$$

- For **inertial particles** in the **Kraichnan model**,

$$x \equiv (\boldsymbol{r}, \boldsymbol{v})\,, \qquad u_t(x) + v_t(x) = \left(\boldsymbol{v}, -\frac{1}{\tau}(\boldsymbol{v} - \boldsymbol{v}_t(\boldsymbol{r}))\right)$$

- For the **Langevin dynamics**,

$$u_t(x) + v_t(x) = -\Gamma \nabla H_t(x) + \Pi \nabla H_t(x) + G_t(x) + \eta_t$$

with Γ a positive matrix, Π an anti-symmetric one, H_t the energy function, G_t an additional force and η_t the white noise with mean zero and covariance $\langle \eta_t \eta_{t'} \rangle = 2\delta(t-t')\,\beta^{-1}\Gamma$

- For the diffusive **hydrodynamical limits** (e.g. of the **SSEP**), the macroscopic particle density $\rho_t(x)$ obeys the continuity equation

$$\partial_t \rho_t + \nabla \cdot j_t = 0$$

with appropriate boundary conditions and

$$j_t^i(x) = -\mathcal{D}^{ij}(\rho_t(x))\,\partial_j \rho_t(x) + \chi^{ij}(\rho_t(x))\,E_j + \eta_t^i(x)$$

with the ρ-dependent small white noise η with mean zero and covariance

$$\langle \eta_t^i(x)\,\eta_s^j(y)\rangle = \epsilon\,\delta(t-s)\,\delta(x-y)\,\chi^{ij}(\rho(x))$$

$\mathcal{D}^{ij}$ and χ^{ij} are the **diffusivity** and the **mobility** matrices, E is the external field, and $\epsilon^{-1} \propto$ number of microscopic particles

The system may be viewed as a **SDE** in the space of densities with

$$u[\rho] = -\nabla\cdot\mathcal{D}(\rho)\nabla\rho - \nabla\cdot\chi(\rho)E\,, \qquad v_t[\rho] = -\nabla\cdot\eta[\rho]$$

Additional elements: extended system $+$ smallness of the noise

Crucial role in what follows will be played by

Time reversal leading to the **backward process**

1. **involution** $(t,x) \longmapsto (T-t, x^*) \equiv (t^*, x^*)$ (may be non-linear)
2. **splitting** $u_t = u_{t,+} + u_{t,-}$ of the deterministic drift

Definition. The backward process x_t is given by the **SDE**

$$\dot{x} = u'_t(x) + v'_t(x)$$

where $u'_t = u'_{t,+} + u'_{t,-}$ with $u'_{t,\pm} = \pm \overset{*}{u}_{t^*,\pm}$

and $v'_t = \pm \overset{*}{v}_{t^*}$ (with whichever sign)

Remark. u_+ transforms as a **vector field**, u_- as a **pseudo-vector field** and v_t as one or the other under the involution

General rule: invert the dissipative terms with the vector rule to avoid that they become anti-dissipative

Examples of time reversals

- In the **deterministic dynamics** one uses usually the **pseudo-vector** rule
- For the **tracer particles**, the usual rule is the **pseudo-vector** one with $\boldsymbol{r}^* = \boldsymbol{r}$ leading to the backward process satisfying

$$\dot{\boldsymbol{r}} = -\boldsymbol{v}_{t^*}(\boldsymbol{r})$$

- For the **inertial particles**, the natural rule is the **vector** one for the friction term $u_{t,+} + v_t = (0, \frac{1}{\tau}(\boldsymbol{v} - \boldsymbol{v}_t(\boldsymbol{r})))$, the **pseudo-vector** one for $u_{t,-} = (\boldsymbol{v}, 0)$, with $(\boldsymbol{r}, \boldsymbol{v})^* = (\boldsymbol{r}, -\boldsymbol{v})$ and the backward equation

$$\dot{\boldsymbol{r}} = \boldsymbol{v}\,, \qquad \dot{\boldsymbol{v}} = \frac{1}{\tau}(\boldsymbol{v} + \boldsymbol{v}_{t^*}(\boldsymbol{r}))$$

- For the **Langevin equation** with $u_{t,+} = -\Gamma\nabla H_t$, $u_{t,-} = \Pi\nabla H_t + G_t$, one gets for the backward process:

$$\dot{x} = -\Gamma\nabla H'_t(x) + \Pi\nabla H'_t(x) + G'_t(x) + \eta'_t$$

where $H'_t(x) = H_{t^*}(x^*)$, $G'_t(x) = -(G_{t^*}(x^*))^*$, $\eta'_t = \pm(\eta_{t^*})^*$

- Among natural time reversals are the ones that take

$$\hat{u}^i_{t,+} = n_t^{-1} d_t^{ij} \partial_j n_t\,, \qquad \hat{u}_{t,-} = \hat{u}_t - \hat{u}_{t,+}$$

were $n_t(x)$ is a density that would be **invariant** if the generator of the process were L_t at all times.

The **generator of the backward process** is then given by

$$L'_t = R\, n_{t^*}^{-1} L^\dagger_{t^*} n_{t^*} R$$

where $(Rf)(x) = f(x^*)$. Up to the involution $x \mapsto x^*$, operator L'_t is the **adjoint** of L_{t^*} w.r.t. the scalar product with density n_{t^*}

Such time reversal (in the stationary setup and with the trivial involution $\rho^* = \rho$) is used for the diffusive **hydrodynamical limits**

Main idea (going back at least to **Onsager-Machlup** 1953):

comparison of fluctuations in forward and backward processes

Let $\big\langle \mathcal{F} \big\rangle_x$ denote the expectation value of a functional $\mathcal{F}$ of the forward process trajectories $[0,T] \ni \mapsto x_t$ starting at $x_0 = x$

Let $\big\langle \mathcal{F} \big\rangle'_x$ denote the same expectation for the backward process

Theorem (**transient fluctuation relation**).

$$\Big\langle \mathcal{F}\, \mathrm{e}^{-\int_0^T \mathcal{J}_t\, dt}\, \delta(x_t - y) \Big\rangle_x \;=\; \Big\langle \mathcal{F}^*\, \delta(x_t^* - x) \Big\rangle'_{y^*}$$

where $\mathcal{F}^*[x_t] = \mathcal{F}[x^*_{t^*}]$ and

$$\mathcal{J}_t[x_t] \;=\; u_{t,+}(x_t) \cdot d_t^{-1}(x_t)\,\big(\dot{x}_t - u_{t,-}(x_t)\big) - (\nabla \cdot u_{t,-})(x_t)$$

Proof. Follows from a combination of the **Girsanov** and **Feynman-Kac** formulae

Interpretation of $\mathcal{J}_t$: **rate of entropy production** in the environment relative to the backward process

For two **normalized densities** $n_0(x)$ and $n_T(x)$ set

$$n'_t(x) = n_{t^*}(x^*)\,\frac{\partial(x^*)}{\partial(x)} \qquad \text{for} \quad t = 0, T$$

Use $n_0(x)$ (resp. $n'_0(x)$) as distributions of the initial points of the forward (resp. backward) process denoting

$$\langle \mathcal{F} \rangle_{n_0} = \int dx\; n_0(x)\,\langle \mathcal{F} \rangle_x\,, \qquad \langle \mathcal{F} \rangle'_{n'_0} = \int dx\; n'_0(x)\,\langle \mathcal{F} \rangle'_x$$

For $\Delta \ln n \equiv \ln n_0(x_T) - \ln n_0(x_0)$, **define**

$$\mathcal{W} = -\Delta \ln n + \int_0^T \mathcal{J}_t\, dt$$

and similarly for $\mathcal{W}' = -\mathcal{W}^*$ using $\Delta \ln n'$ and the backward process

Immediate **Corollaries** of **Theorem**:

- **Detailed fluctuation relation**:

$$\left\langle \mathcal{F}\,\mathrm{e}^{-\mathcal{W}} \right\rangle_{n_0} \;=\; \left\langle \mathcal{F}^* \right\rangle_{n'_0}$$

- **Crooks relation**: taking $\mathcal{F} = \delta(\mathcal{W} - W)$ implies that the

$$\mathrm{e}^{-W}\, p_T(W) \;=\; p'_T(-W)$$

where $p_T(W)$ (resp. $p'_T(W)$) is the **PDF** of $\mathcal{W}$ (resp. $\mathcal{W}'$):

$$p_T(W) \equiv \langle \delta(\mathcal{W} - W) \rangle_{n_0}\,, \qquad p'_T(W) \equiv \langle \delta(\mathcal{W}' - W) \rangle'_{n'_0}$$

- **Jarzynski equality**: taking $\mathcal{F} \equiv 1$ implies that

$$\left\langle \mathrm{e}^{-\mathcal{W}} \right\rangle_{n_0} \;=\; 1$$

Entropy balance:

If n_T is obtained from n_0 by the dynamical evolution then $-\Delta \ln n$ may be interpreted as the change of instantaneous entropy of the system and $\mathcal{W}$ becomes the **total entropy production**.

The inequality

$$\langle \mathcal{W} \rangle_{n_0} \geq 0$$

that follows from the Jarzynski equality via the Jensen inequality has then the interpretation of the **2$^{\mathrm{nd}}$ Law of Thermodynamics**

Remark: Keep in mind that $\mathcal{W}$ depends on the choice of the backward process and of the initial distributions. Different choices lead to different notions of entropy production

Case of stationary dynamics

For large times T, the **PDF** $p(W)$ may take the **large deviations** form

$$p_T(Tw) \;\approx\; \mathrm{e}^{-T\,\zeta(w)}$$

and similarly for $p'_T(Tw)$. The Crooks relation implies then that

$$\zeta(w) + w \;=\; \zeta'(w)$$

If the forward and backward processes have the same distribution (e.g. with the vector rule for the drift reversal and $x^* \equiv x$) then $\zeta' = \zeta$
$\Rightarrow$ the **Gallavotti-Cohen symmetry** of the **rate function** ζ.

Remark. If $n(x)$ is the stationary density and $\ln n(x)$ is bounded (e.g. for the process in a bounded domain) then $\mathcal{W}/T$ and $\frac{1}{T}\int\limits_0^T \mathcal{J}_t\, dt$, differing by a boundary term $\frac{1}{T}\Delta \ln n$, will have the same large deviations

Relation to the **empirical density** and **empirical current** defined by

$$n_T(x) \;=\; \frac{1}{T}\int_0^T \delta(x-x_t)\,dt\,, \qquad j_T(x) \;=\; \frac{1}{T}\int_0^T \delta(x-x_t)\,\dot{x}_t\,dt$$

The large deviations of $\frac{1}{T}\int_0^T \mathcal{J}_t\,dt$ may be obtained from those of (n_T, j_T) governed by the rate functional equal to

$$I[n,j] \;=\; \frac{1}{4}\int \big(j(x)-j_n(x)\big)\cdot d(x)^{-1}\big(j(x)-j_n(x)\big)\,n(x)^{-1}\,dx$$

if $\nabla\cdot j\equiv 0$ and to $+\infty$ otherwise, where $j_n^i = (\hat{u}^i - d^{ij}\partial_j)n$ is the **probability current** associated to the density n. Since

$$\frac{1}{T}\int_0^T \mathcal{J}_t\,dt = \int \big[u_+\cdot d^{-1}j_T - (\hat{u}_+\cdot d^{-1}u_- + \nabla\cdot u_-)n_T\big](x)\;dx \;\equiv\; w[n_T, j_T]\,,$$

one has:

$$\zeta(w) \;=\; \min_{(n,j)\in\mathcal{A}_w} I(n,j)$$

where $\mathcal{A}_w \;=\; \{\,(n,j)\;|\;\nabla\cdot j\equiv 0 \;\text{ and }\; w = w[n,j]\,\}$

The stationary fluctuation relation $\zeta(w)+w=\zeta'(-w)$ follows from the one for the rate functionals I :

$$I[n,j]\,+\,w[n,j]\;=\;I'[n^*,-j^*]$$

where $n^*(x)=n(x^*)\,\frac{\partial(x^*)}{\partial(x)}$ and $j^{*\,i}(x)=\frac{\partial x^i}{\partial x^{*\,k}}\,j^k(x^*)\,\frac{\partial(x^*)}{\partial(x)}$

Remark. Calculation of large deviations rate functions and even their existence is often not granted, as simple examples show.

Their study for the hydrodynamical limits of stochastic lattice gases has been a subject of intensive activity (see the courses of **Jona-Lasinio, Derrida, Kurchan,** ...)

Multiplicative fluctuation relations

The theory applies to diffusion processes derived from the original one

Example:

$$\dot{x}^i = u^i_t(x) + v^i_t(x)\,, \qquad \dot{X}^{ij} = (\partial_k u^i_t)(x)\, X^k_{\ j} + (\partial_k v^i_t)(x)\, X^k_{\ j}$$

Matrix $X(t)$ propagates infinitesimal separations δx_t between two trajectories of the process x_t:

$$\delta x_t = X(t)\,\delta x_0 \qquad \text{if} \qquad X(0) = 1$$

For the **tangent process** (x_t, X_t), using the pseudo-vector rule to revert the drift and the involution $(x, X)^* \equiv (x^*, X^*)$ with $(X^*)^i_{\ j} = \frac{\partial x^{*\,i}}{\partial x^k} X^k_{\ j}$, one obtains

$$\mathcal{J}_t[x_t, X_t] = -(d+1)\frac{d}{dt}\,\ln\det(X_t)$$

and the **transient fluctuation relation** takes the form

$$\det(X)\left\langle \delta(x_t - y)\,\delta(X_t - X)\right\rangle_{(x,1)} = \left\langle \delta(x^*_t - x)\,\delta(X^{*\,-1}_t - X)\right\rangle'_{(y^*,1^*)}$$

Define the **stretching rates** $\sigma_t^1 \geq \cdots \geq \sigma_t^d$ as the eigenvalues of the matrix $\frac{1}{2t}\ln(X_t^{tr} X_t)$. If $x \mapsto x^*$ preserves the Euclidean metric then

$$\mathrm{e}^{T\sum\limits_i \sigma^i} \left\langle \delta(x_t - y)\, \delta(\vec{\sigma}_T - \vec{\sigma}) \right\rangle_{(x,0)} = \left\langle \delta(x_t^* - x)\, \delta(\vec{\sigma}_T + \overleftarrow{\sigma}) \right\rangle'_{(y^*,0)}$$

where $\overleftarrow{\sigma} = (\sigma^d, \ldots, \sigma^1)$. In the stationary large deviation regime with

$$\left\langle \delta(x_t - y)\, \delta(\vec{\sigma}_T - \vec{\sigma}) \right\rangle_{(x,0)} \approx \mathrm{e}^{-TZ(\vec{\sigma})}$$

this gives the **stationary multiplicative fluctuation relation**

$$Z(\vec{\sigma}) - \sum_i \sigma^i = Z'(-\overleftarrow{\sigma})$$

For Lagrangian tracers in Kraichnan velocities with vanishing mean, $Z'(\vec{\sigma}) = Z(\vec{\sigma})$

For inertial particles, $\sum \sigma^i = -\frac{d}{\tau}$ but $Z'(\vec{\sigma}) \neq Z(\vec{\sigma})$ and the Gallavotti-Cohen relation is deformed to (**Fouxon-Horvai** 2007) :

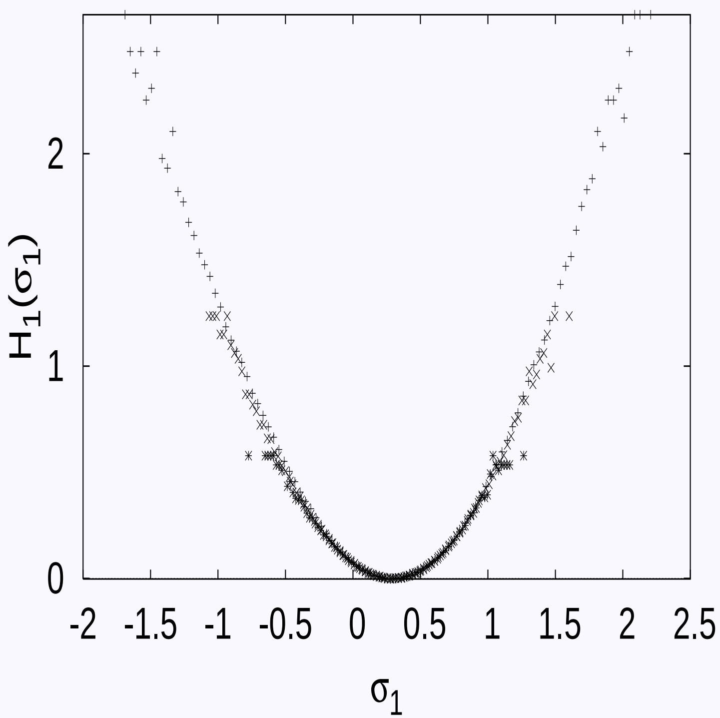
$$Z(\vec{\sigma}) = Z(-\overleftarrow{\sigma} - \tfrac{1}{\tau}\vec{1})$$

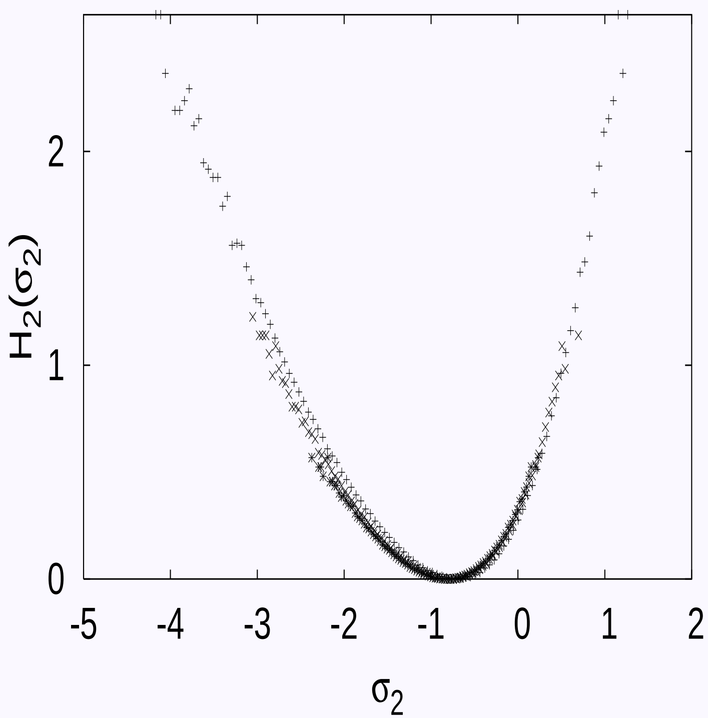
- $Z(\vec{\sigma})$ takes its (vanishing) minimal value at $\vec{\sigma} = \vec{\lambda}$, where $\vec{\lambda}$ is the vector of the **Lyapunov exponents**, but it contains more information

- $Z(\vec{\sigma})$ is analytically calculable in the Kraichnan model in some cases via relations to integrable models (**Bernard-Kupiainen-K.G.** 1997, **Delannoy-Chetrite-K.G** 2006)

- $Z(\vec{\sigma})$ is important for turbulent transport since it determines:
  - rate of decay of moments of transported scalar
  - rate of growth of density and magnetic field fluctuations
  - multi-fractal dimensions of attractor for tracers in compressible flows and for inertial particles
  - polymer stretching in presence of turbulence

- $Z(\vec{\sigma})$ becomes accessible numerically in simulations of realistic flows and even experimentally





from **Boffeta-Davoudi-De Lillo**, Europhys. Lett., **74**, 62-68 (2006)
(numerical results for two-dimensional surface flows)

Conclusions

- The setup of diffusion processes permits to discuss in a uniform way fluctuations in models of non-equilibrium statistical mechanics and of turbulent transport
- Fluctuation relations in such systems compare the statistics of fluctuations of quantities related to entropy production between forward and backward processes
- In stationary systems they induce relations between the rate functions of large deviations governing the long time asymptotics of fluctuations
- Applied to tangent processes, the fluctuation relations induce their multiplicative extensions
- Further analytic calculations, simulations and experimental measurements of fluctuation statistics in concrete situations are needed