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Article

# Is Turbulence a State of Maximum Energy Dissipation?

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**Abstract:** Turbulent flows are known to enhance turbulent transport. It has then even been suggested that turbulence is a state of *maximum energy dissipation*. In this paper, we re-examine critically this suggestion at the light of several recent works around the Maximum Entropy Production principle (MEP) that has been used in several out-of-equilibrium systems. We provide a set of 4 different optimization principles, based on maximization of energy dissipation, entropy production, Kolmogorov-Sinai entropy and minimization of mixing time, and study the connection between these principles using simple out-of-equilibrium models describing mixing of a scalar quantity. We find that there is a chained-relationship between most probable stationary states of the system, and their ability to obey one of the 4 principle. This provides an empirical justification of the Maximum Entropy Production principle in this class of systems, including some turbulent flows, for special boundary conditions. Otherwise, we claim that the minimization of the mixing time would be a more appropriate principle. We stress that this principle might actually be limited to flows where symmetry or dynamics impose pure mixing of a quantity (like angular momentum, momentum or temperature). The claim that turbulence is a state of maximum energy dissipation, a quantity intimately related to entropy production, is therefore limited to special situations that nevertheless include classical systems such as Shear flows, Rayleigh Benard convection and von Karman flows, forced with constant velocity or temperature conditions.

**Keywords:** Maximum Entropy Production; Turbulence; Kolmogorov-Sinai entropy

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## 1. Introduction: Turbulence as a maximum Energy Dissipation State?

A well-known feature of any turbulent flow is the Kolmogorov-Richardson cascade by which energy is transferred from scale to scale until scales at which it can be dissipated. This cascade is a non-linear, non-equilibrium process. It is believed to be the origin of the significant enhancement of dissipation observed in turbulent flow, often characterized via the introduction of a *turbulent viscosity*.

It has then sometimes been suggested that turbulence is a state of *maximum energy dissipation*. This principle inspired early works by Malkus [1,2] or Spiegel [3] to compute analytically the heat or momentum profiles in thermal boundary layers or linear shear flows. While there were many

27 criticisms about this principle, there are a few experimental situation where this principle seems to  
28 work. A good example is provided by the von Karman flow. This flow is generated by two-counter  
29 rotating impellers inside a cylindrical vessel filled e.g. with water (see Figure 1). The impellers  
30 produce a source of angular momentum at the top and bottom of the vessel, angular momentum  
31 that is then transferred and mixed within the flow throughout the turbulent motions [4], in analogy  
32 with heat transferred through a Rayleigh-Benard cell. For most impellers, the resulting mean large  
33 scale stationary motion is the superposition of a two-cell azimuthal motion, and a two cell poloidal  
34 motion bringing the flow from the top and bottom end of the experiment towards its center plane  
35  $z = 0$  (see Figure 1). This mean flow is thus symmetrical with respect to the plane  $z = 0$ . For some  
36 types of impellers, however, this symmetrical state is unstable, and bifurcates after a certain time  
37 towards another state that breaks the system symmetry [5,6]-see Figure 2. This state corresponds to  
38 a global rotation in the direction of either the top or the bottom impeller. The energy dissipation  
39 corresponding to either one of these 3 states can be measured through monitoring of the torque  
40 applied to the impellers by the flow. When monitored during a bifurcation (see Figure 3), this energy  
41 dissipation displays a jump (by a factor 4) at the moment of the bifurcation from the symmetrical state  
42 towards either one of the non-symmetrical states. Once the system is in the bifurcated state, it never  
43 bifurcates back towards the symmetrical state, indicating that the most stable state is the state with  
44 larger dissipation.

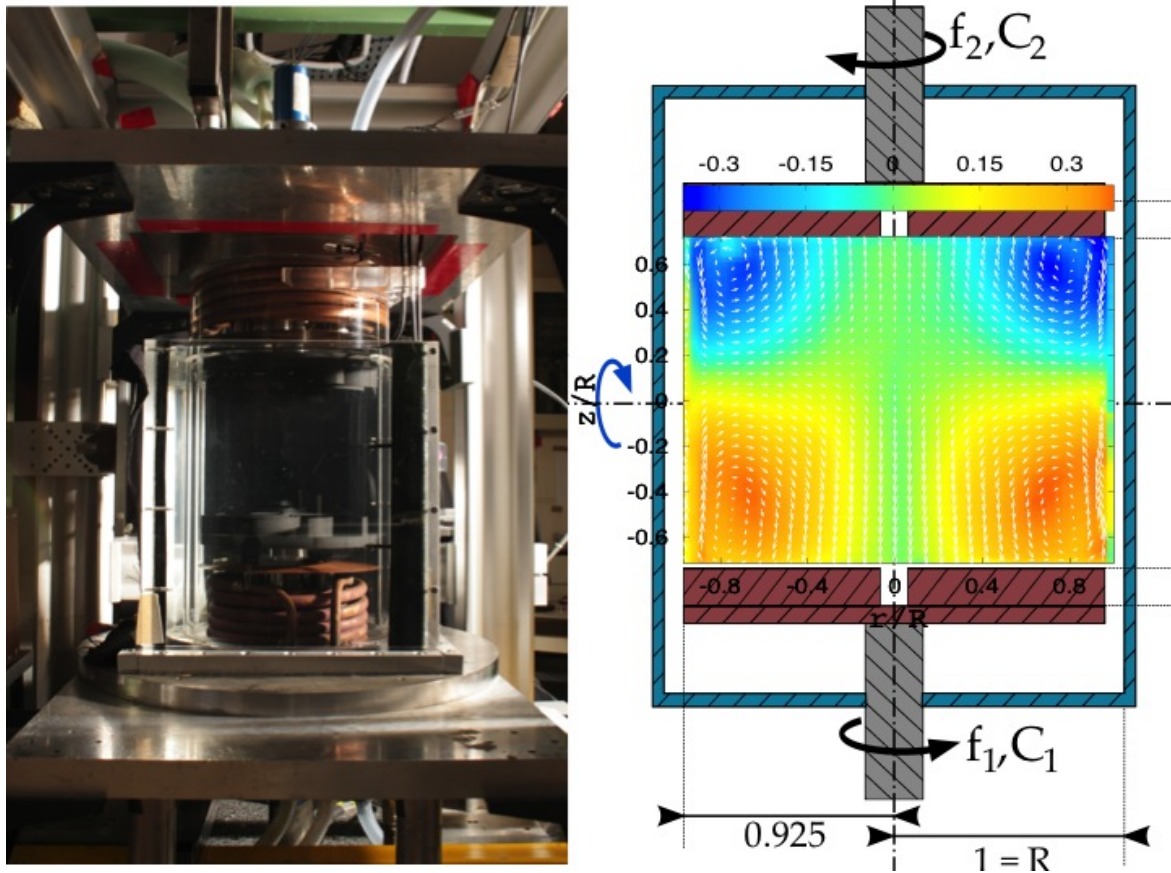
45 This observation is in agreement with a general principle inspired from Malkus principle, that could  
46 be formulated as follow:

47 *Principle A: In certain non-equilibrium systems with coexistence of several stationary state, the most*  
48 *stable one is that of Maximum Energy Dissipation.*

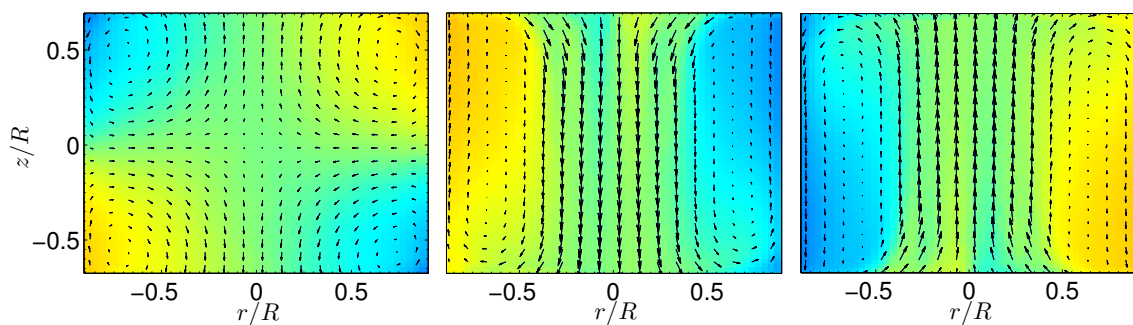
49  
50 This principle is of course very appealing. There are however no derivation of it from any first  
51 principles, and we are not aware of any theories that could lead to its proof (while there are probably  
52 many immediate counter-example that can be provided). If it is true or approximately true for  
53 some types of flows (like the von Karman flow, or the Rayleigh-Benard flow or the plane Couette  
54 flow), it may then lead to interesting applications allowing the computation of mean velocity or  
55 temperature profile without the need to integrate the whole Navier-Stokes equations. A way to  
56 proceed with its justification is to transform it into an equivalent principle, that uses notions more  
57 rooted in non-equilibrium physics. Indeed, energy dissipation is not a handful quantity to work with  
58 in general, because of its dependence on the small scale processes that produce it. In general, energy  
59 dissipation is a signature of entropy production. The connection between energy dissipation and  
60 entropy production was heuristically made by Lorenz [7] and theoretically discussed in nonlinear  
61 chemical thermodynamics by Dewar [8] and Moroz [9,10]. This last notion seems more appealing to  
62 work with and a first natural step is to modify slightly the principle A into a more appealing version  
63 as:

64 *Principle B: In certain non-equilibrium systems with coexistence of several stationary state, the most*  
65 *stable one is that of Maximum Entropy Production (MEP).*

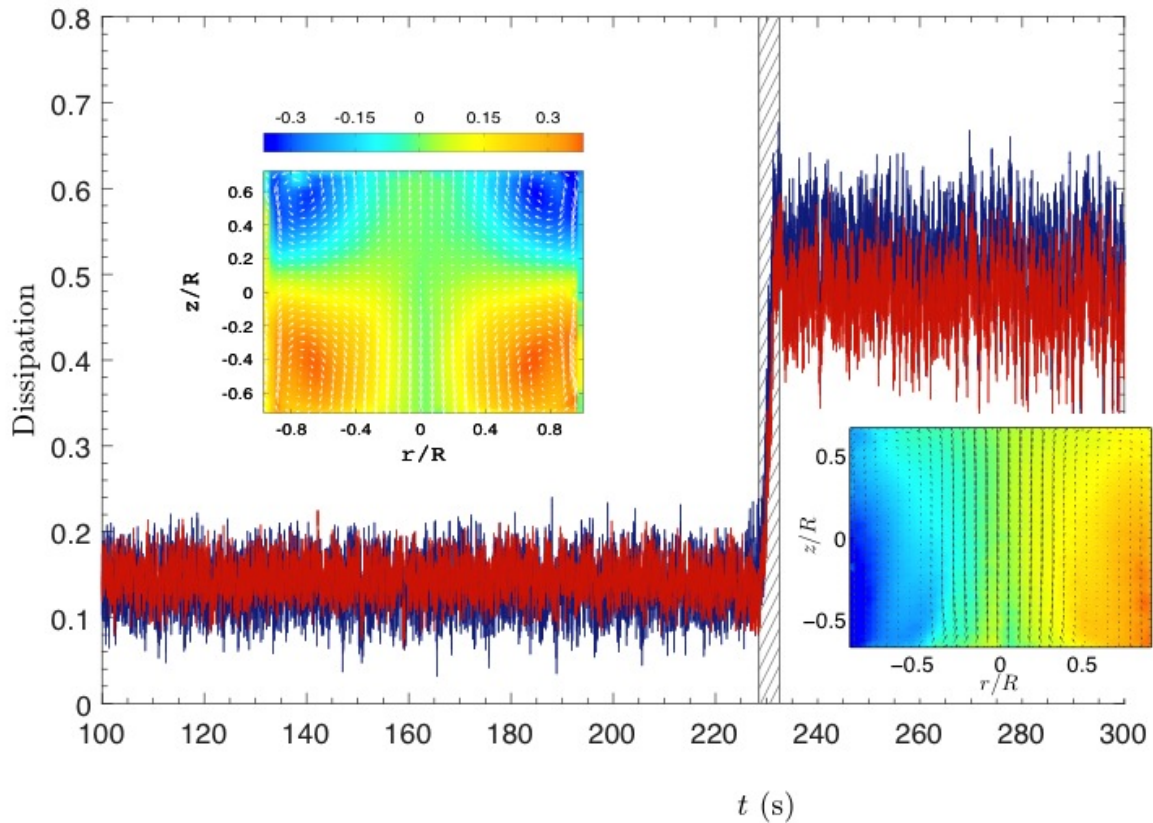
66  
67 From the point of view of non-equilibrium physics, this principle appears as a counterpart of the well  
68 known principle of Maximum Entropy that governs stability of equilibria in statistical physics, the  
69 analog of equilibria here being the stationary states. This principle was discovered by Ziegler [11,12]  
70 and it is sometimes referred to as the Ziegler's principle. It has found several applications in climate  
71 dynamics: first it was used by Paltridge [13] to derive a good approximation of the mean temperature  
72 distribution in the mean atmosphere of the Earth. This approach has been extend to more exhaustive  
73 climate models by Herbert [14]. Kleidon et al. [15] used an atmospheric general circulation model to  
74 show that MEP states can be used as a criterion to determine the boundary layer friction coefficients.



**Figure 1.** Von Karman experiment. The flow is generated inside a cylindrical vessel through counter-rotation of two impellers. The impellers inject angular-momentum at the top and the bottom, inducing a large scale circulation inside the flow. At low Reynolds numbers, the circulation is symmetrical with respect to a  $\pi$ -rotation around a horizontal axis through the origin (blue arrow). One can impose the torque  $C_i$  or the rotation frequency  $f_i$  to the flow, generating different turbulent regimes. The right picture shows a representation of the mean velocity fields in a plane passing for the axis of the cylinder (arrows) and orthogonal to this plane (colorscale in m/s), obtained by averaging several thousands instantaneous fields. (Pictures courtesy Brice Saint-Michel).



**Figure 2.** The 3 stationary states of the von Karman flow: left: The symmetric state. Middle and right: the two bifurcated states, that are symmetric to each other with respect to a  $\pi$ -rotation along an axis going through the rotation axis [5,6]. Color coding as in Figure 1.



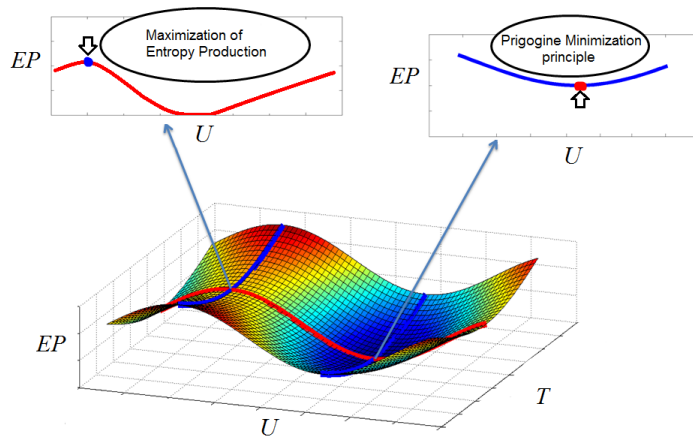
**Figure 3.** Spontaneous bifurcation in the von Karman flow: the flow, initially started in a symmetrical state, bifurcates after a certain time toward a bifurcated state, that produces a 4 times larger dissipation [5]. The dissipation is measured through monitoring of the torque, applied on each propeller, by the turbulent flow. This flow being turbulent, the resulting torque is widely fluctuating around a mean value, characterizing the dissipation. Colour coding of the flow as in Figure 1. Colour coding of the dissipation is blue for the dissipation measured on the lower propeller, and red for the dissipation measured on the upper-propeller. The total dissipation is the sum of the two contributions.

75 MEP seems also a valuable principle to describe planetary atmospheres, as those of Mars and Titan  
76 where it has been used to determine latitudinal temperature gradients [16]. MEP have been also  
77 applied to several geophysical problems: to describe thermally driven winds [17] and convection[18],  
78 and to oceanic circulation [19]. A detailed overview on the usefulness of MEP in climate science can  
79 be found in [20,21] and references therein. It is therefore interesting to evaluate the soundness of this  
80 principle and understand its limitation and its possible improvements, to extend as possible the scope  
81 of its applications. The usual path to prove the validity of a principle is to provide some rigorous  
82 demonstration of the principle itself. This task has been attempted without convincing results in  
83 the past years [8,22,23]. In the absence of any theory of out-of-equilibrium systems, we may turn to  
84 equilibrium theory as a guide to find a path for justification of the selection of stationary states. In  
85 equilibrium systems or conceptual models, this selection can be studied using the dynamical systems  
86 theory, where other quantities than thermodynamics entropy are relevant. One of this quantity is the  
87 Kolmogorov Sinai Entropy (KSE) [24], which is indeed different from the thermodynamic one. The  
88 KSE appears a good candidate for the selection of preferred metastable states because it is related to  
89 the concept of mixing time [25]. The goal of this paper is therefore to show that MEP principle could  
90 find a justification in a linked relationship which involves studying the connections among MEP, KSE  
91 and mixing times. The paper follow this structure: after discussing the relation between MEP and  
92 the Prigogine minimization principle (section II), we connect MEP and maximum KSE in conceptual  
93 models of turbulence (section III). In section IV we establish the link between maximum KSE and  
94 mixing times for Markov chains. Then, we summarize the results and discuss the implications of our  
95 findings.

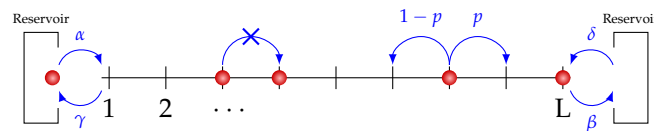
## 96 2. Maximization or Minimization of Entropy production?

97 At first sight, Principle B appears in conflict with an established result of Prigogine, according to  
98 which the stationary states of a system close to equilibrium are states with *minimum* entropy  
99 production. In fact, both principles can be reconciled if Principle B is viewed as a MaxMin, principle:  
100 Martyushev et al. [26] and Kleidon [21] suggest that Prigogine's principle select the steady state  
101 of minimum entropy production compared to transient states. For a steady-state condition, the  
102 minimum entropy production principle does not give any further information if many steady state  
103 conditions are possible given the imposed boundary conditions. To provide a simple example, let us  
104 consider a system characterized by two parameters,  $T$  and  $U$ , where  $T$  controls the departure from  
105 equilibrium and  $U$  labels an additional constraint of the system, allowing the existence of several  
106 stationary states at a given  $T$  (see Figure 4). In our von Karman system,  $T$  could for example label  
107 the velocity fluctuations, and  $U$  the angular momentum transport. In the  $T$  direction, application  
108 of the Prigogine principle selects the value of  $T$  corresponding to the stationary state. When there  
109 are several possible stationary state, the Principle B then selects the most stable state as the one with  
110 the largest entropy production, thereby fixing the corresponding value of  $U$ . This was precisely the  
111 procedure followed by Paltridge.

112 On the other hand, it appears that the stability of the stationary state may depend on boundary  
113 conditions. For example, Niven [27] or Kawazura and Yoshida [28] provide explicit examples of  
114 out-of-equilibrium systems, in which the entropy production is *sl* maximized for fixed temperature  
115 boundary conditions, while it is *minimized for fixed heat flux* boundary conditions. In the  
116 experimental von Karman system discussed in Section 1, we observe a similar phenomenon: for fixed  
117 propeller velocities, the selected stationary state is the one of maximum dissipation. However, when  
118 one changes the boundary conditions into fixed applied torque at each propeller, the stationary state  
119 regime disappears and is replaced by a dynamical regime, in which the system switches between  
120 different meta-stable states of low and high energy dissipation [6]. This case is discussed in more  
121 detail in Section 6. It shows however that we cannot trust the Maximum Entropy Production principle  
122 blindly, and must find ways to understand why and when it works, using tools borrowed from



**Figure 4.** Illustration of the relation between maximization of entropy production  $EP$  and Prigogine principle: the system is set out of equilibrium by the parameters  $T$  and  $U$ .  $T$  controls the departure from equilibrium and  $U$  labels an additional constraint of the system. In the  $T$  direction, application of the Prigogine principle selects the value of  $T$  corresponding to the stationary state, where MEP selects the one with largest  $EP$  in the  $U$  direction.



**Figure 5.** The dynamical rules of the toy model of scalar transport: the particle can jump to the left or to the right with probabilities denoted by  $p$ . At both end, two reservoirs sets the flux of incoming or outgoing particles. The particle can be a boson (several particles per box are allowed), in which case the process is called zero-range process (ZRP). When the particle is a fermion, jump towards a box that is already occupied are forbidden. The corresponding process is called asymmetric exclusion process (ASEP).

123 non-equilibrium theories. A justification has been attempted [8], and dismissed [22,23], following the  
 124 ideas of Jaynes that non-equilibrium systems should be characterized by a probability distribution  
 125 on the trajectories in phase space, instead of just the points in phase space at equilibrium. A more  
 126 pragmatic way to evaluate the validity of Principle B is to consider its application to toy models of  
 127 non-equilibrium statistics, that mimics the main processes at work in the von Karman flow, and that  
 128 can guide us on a way to a justification (or dismissal). This is the topic of the next section.

### 129 3. From Maximum entropy production to Maximum Kolmogorov-Sinai entropy in toy models of 130 turbulence

#### 131 3.1. From passive scalar equation to Markovian box models

In the von Karman flow, angular momentum is transported from the vessel ends towards the center. In Rayleigh-Benard, the temperature is transported from the bottom to the top plates. In shear flows, the linear momentum is transported from one side to the other. On Earth, the heat is transported from the equator towards the pole. All this system in which Principle B seems to provide a non-trivial answer have then in common that they deal with the transport of a scalar quantity  $T$  by a given velocity field  $u(x, t)$ , and that may be sketched as:

$$\partial_t T + u \nabla T = \kappa (\nabla)^2 T, \quad (1)$$

132 with appropriate boundary conditions. Here  $\kappa$  is the diffusivity. To transform this process into a  
 133 tractable toy model, we stick to a one dimensional case and divide the accessible space  $\ell$  into  $L$   
 134 boxes. We impose the boundary conditions through two reservoirs located at each end of the chain  
 135 (mimicking e.g. the top and bottom propeller or solar heat flux at pole and equator). The boxes  
 136 contains bosonic or fermionic particles that can jump in between two adjacent boxes via decorrelated  
 137 jumps (to the right or to the left) following a 1D Markov dynamics governed by a coupling with  
 138 the two reservoirs imposing a difference of chemical potential at the ends. The different jumps are  
 139 described as follow. At each time step a particle can jump right with probability  $pw_n$  or jump left with  
 140 probability  $(1-p)w_n$ .  $w_n$  is a parameter depending on the number of particles inside the box and  
 141 on the nature of particles. Choices of different  $w_n$  give radically different behaviors. For fermionic  
 142 particles, it prevents a jump on to a site, if this site is already occupied by a particle. The corresponding  
 143 process is called Asymmetric Exclusion Process (ASEP). For boson,  $w_n = 1$  and the process is called  
 144 Zero Range Process (ZRP). At the edges of the lattice the probability rules are different: at the left  
 145 edge a particle can enter with probability  $\alpha$  and exit with probability  $\gamma w_n$  whereas at the right edge a  
 146 particle can exit with probability  $\beta w_n$  and enter with probability  $\delta$ .

147 Without loss of generality, we may consider only  $p \geq 1/2$  which corresponds to a particle flow  
 148 from the left to the right and note  $U = 2p - 1$ . After a sufficiently long time the system reaches a  
 149 non-equilibrium steady state, with a well defined density profile (or fugacity profile) across the boxes  
 150 ranging between  $\rho_a$ , the density of the left reservoir and  $\rho_b$ , the density of the right reservoir, given by  
 151  $\rho_a = \alpha(\gamma + \epsilon\alpha)$  and  $\rho_b = \delta(\beta + \epsilon\delta)$ , where  $\epsilon = 1$  for ASEP (fermion) and  $\epsilon = -1$  for ZRP (boson). In  
 152 the sequel, we fix  $\gamma + \alpha = 1$  and  $\beta + \delta = 1$ , and denote  $\Delta T = \rho_a - \rho_b$  the parameter that measures the  
 153 balance between the input rate of the left reservoir (the equivalent of the heat or momentum injection),  
 154 and the removal rate of the right reservoir (the equivalent of the heat or momentum dissipation). Once  
 155  $\beta$  (say),  $\Delta T$  are fixed, we can compute all the other parameter  $\alpha$ ,  $\gamma$  and  $\delta$  of the model. In the sequel,  
 156 we fix  $\beta = 0.75$ , and vary  $\Delta T$  and/or  $U$ .

Taking the continuous limit of this process, it may be checked that the fugacity  $Z = \rho/(1 + \rho)$   
 of stationary solutions of a system consisting of boxes of size  $\frac{1}{L}$  follow the continuous equation  
 [29]:

$$U \frac{\partial Z}{\partial x} - \frac{1}{2L} \frac{\partial^2 Z}{\partial x^2} = 0, \quad (2)$$

corresponding to stationary solution of a passive scalar equation with velocity  $U$  and diffusivity  $\frac{1}{2L}$ .  
 Therefore, the fugacity  $Z$  is a passive scalar obeying a convective-diffusion equation. We thus see  
 that  $U = 0$  corresponds to a purely conductive regime whereas the larger  $U$  the more convective the  
 regime. This toy model therefore mimics in the continuous limit the behavior of scalar transport in the  
 von Karman, Rayleigh-Bénard, Couette or Earth system we are trying to understand. The toy model  
 is a discrete Markov process with  $2^L$  states. It is characterized by its transition matrix  $P = (p_{ij})$  which  
 is irreducible. Thus, the probability measure on the states converges to the stationary probability  
 measure  $\mu = (\mu_{1_{stat}}, \dots, \mu_{2^L_{stat}})$  which satisfies:

$$\mu_{i_{stat}} = \sum_{j=1}^{2^L} \mu_{j_{stat}} \cdot p_{ji} \quad \forall i \in \llbracket 1, 2^L \rrbracket. \quad (3)$$

157 This Markov property makes our model simple enough so that exact computations are analytically  
 158 tractable and numerical simulations are possible up to  $L = 10$  (ASEP model) to  $L = 1000$  (ZRP  
 159 model) on a laptop computer. The idea now is to apply the Principle B in these toy models, and see  
 160 what useful information we can derive from it.

161

162 3.2. Maximum Entropy production in Zero Range and ASymmetric Exclusion Process

163 We turn to the definition of entropy production in our toy model system. For a macroscopic system  
 164 subject to thermodynamic forces  $X_i$  and fluxes  $J_i$ , the thermodynamic entropy production is given by:  
 165 [30,31]:

$$\sigma_{thermo} = \sum_i J_i X_i \quad (4)$$

166 The fluxes to consider for a diffusive particles model are fluxes of particles and the thermodynamic  
 167 forces can be written  $X = \Delta(-\frac{\nu}{T})$  where  $T$  is the temperature and  $\nu$  the chemical potential  
 168 proportional to  $\log(\rho)$  for an ideal gas [30]. So, as the temperature is here fixed, the thermodynamic  
 169 Entropy production of a given stationary state takes the form:

$$\sigma_{thermo} \propto \sum_{i=1}^L J_i (\log(\rho_i) - \log(\rho_{i+1})) = J \cdot (\log(\rho_1) - \log(\rho_L)) \quad (5)$$

where  $\rho$  is the stationary density distribution and  $J = J_i$  the particle fluxes in the stationary state,  
 where all fluxes become equal and independent on the site.  $\rho$  and  $J$  are both (nonlinear) function of  
 $U$ . It is easy to show [32] that this definition is just the continuous limit of the classical thermodynamic  
 entropy production in an ideal gas, that reads:

$$\sigma_{thermo} = - \int_{A_+}^{B_-} J(x,t) \frac{\partial \log(\rho(x,t))}{\partial x} dx \quad (6)$$

In the case of bosonic particles (ZRP model), this entropy production takes an compact analytical  
 shape in the (thermodynamic) limit  $L \rightarrow 0$  [33]:

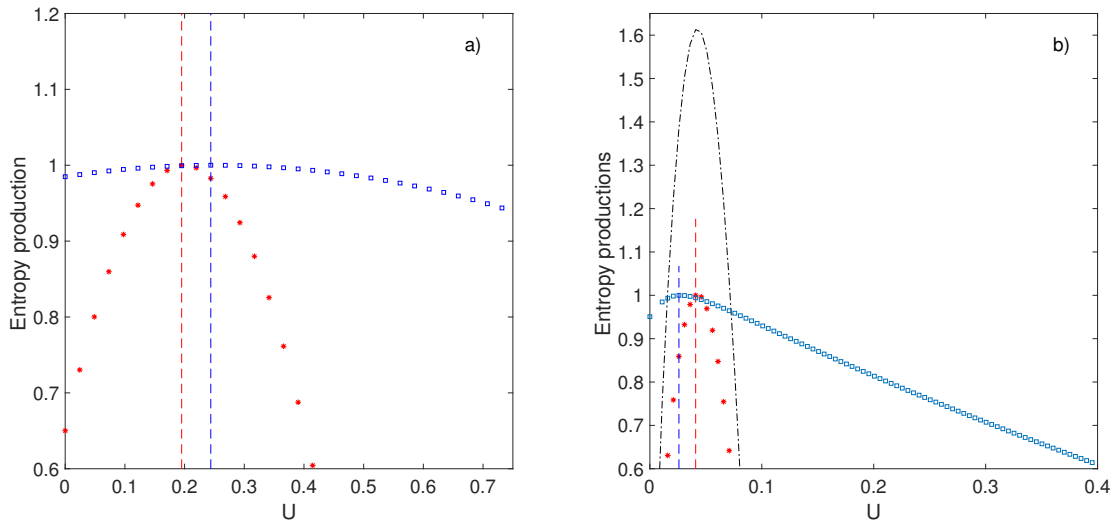
$$\sigma(U) = \frac{\alpha U}{U + \gamma} \left( \log\left(\frac{\alpha}{U + \gamma - \alpha}\right) - \log\left(\frac{(\alpha + \delta)U + \gamma\delta}{U(\beta - \alpha - \delta) + \beta\gamma - \gamma\delta}\right) \right) \quad (7)$$

170 Because  $U = 2p - 1 \geq 0$  the entropy production is positive if and only if  $\rho_a \leq \rho_b$ . This means that  
 171 fluxes are in the opposite direction of the gradient. We remark than if  $U = 0$  then  $\sigma(U) = 0$ . Indeed  
 172  $J$  is proportional to  $U$  in this model. Moreover,  $\sigma(U)$  is zero also when  $\rho_1 = \rho_L$ . This happens when  
 173  $U$  increases,  $\rho_a(U)$  decreases and  $\rho_b(U)$  increases till they take the same value. Thus it exists  $U$ , large  
 174 enough, for which  $\sigma(U) = 0$ . Between these two values of  $U$  the entropy production has at least one  
 175 maximum. By computing numerically the entropy production, we observe in fact that it is also true  
 176 for the fermionic particles, even though we cannot prove it analytically. This is illustrated in Figure 6  
 177 for  $L = 100$  (ZRP) and  $L = 10$  (ASEP).

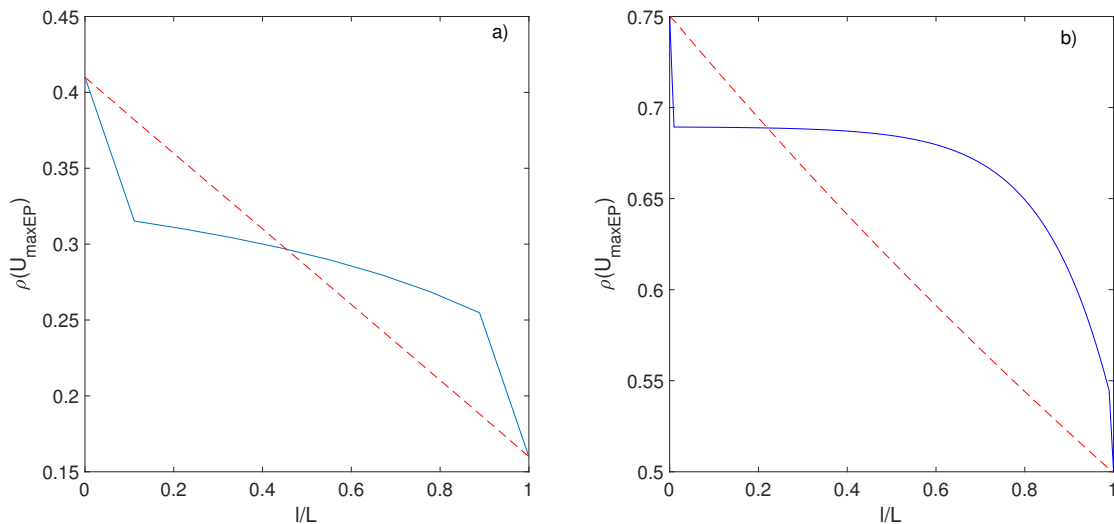
The value of  $U_{maxEP}(T)$  at which this maximum occurs depends on the distance to equilibrium of the  
 system, characterized by the parameter  $\Delta T = \alpha - \delta$ . In the case of the ZRP model, it can be computed  
 as [33]:

$$U_{maxEP,ZRP} = \frac{\Delta T}{4M\alpha} + 3 \frac{\Delta T^2(\alpha + 1)}{8M^2\alpha^2(\alpha - 1)} + o((\Delta T)^2), \quad (8)$$

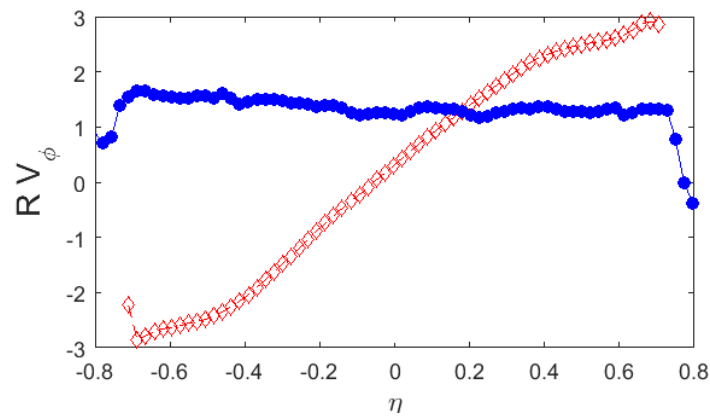
178 where  $M = (1 + 2\rho_a)(1 + 2\rho_b)$ . This means that at equilibrium ( $\Delta T = 0$ ,  $\rho_a = \rho_b$ ), the maximum  
 179 is attained for  $U = 0$ , i.e. the symmetric case. Numerical simulations of the ASEP system suggest  
 180 that this behavior is qualitatively valid also for fermionic particles: the entropy production displays  
 181 a maximum, that varies linearly in  $\Delta T$ . Such behavior therefore appears quite generic of this class of  
 182 toy model. When the system is close to equilibrium ( $\Delta T \ll 1$ ), the maximum is very near zero, and,  
 183 the density profile is linear, corresponding to a *conductive* case. When the system is out-of-equilibrium  
 184 ( $\Delta T \geq 0$ ) the maximum is shifted towards larger values of  $U > 0$ , corresponding to a *convective state*,  
 185 with flattened profile. An example is provided in Figure 7 for the ZRP and ASEP model.



**Figure 6.** Entropy productions as a function of  $U$  for  $\beta = 0.75$  and  $\Delta T = 0.25$  for two toys models. Red stars: Thermodynamic entropy production  $\sigma(U)$ ; blue squares: Kolmogorov-Sinai entropy  $h_{KS}(U)$ . The location of the maxima are denoted by vertical dashed line (red for  $\sigma(U)$ ; and blue for  $h_{KS}(U)$ ). a) Case  $L=10$  ASEP (fermion) ; b) Case  $L=100$  ZRP (boson) . The dot-dashed line is the asymptotic law for  $\sigma(U)$  given by Eq. (7).



**Figure 7.** Profiles of density profiles (blue line) corresponding to models with  $U = U_{maxEP}$  for  $\beta = 0.75$  and  $\Delta T = 0.25$  for two toys models. The red dashed line is the density profile obtained at  $U = 0$ , i.e. in the *conductive case*. a) Case  $L=10$  ASEP (fermion) ; b) Case  $L=100$  ZRP (boson)



**Figure 8.** Profiles of angular momentum  $RV_\phi$  as a function of the height from the central plane  $\eta$  in the von Karman laboratory experiment. Blue symbols with line: in the *bifurcated* state with higher energy dissipation. Red line with symbols: in the symmetric state.

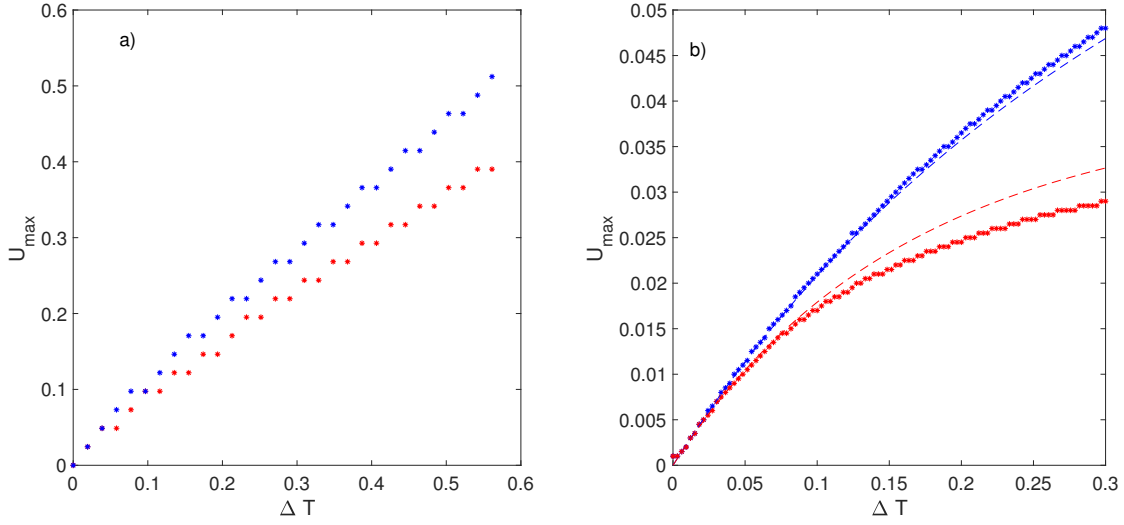
186 Our toy models are examples of systems with deviation from equilibrium (labelled by  $\Delta T$ ), admitting  
 187 several stationary states (labelled by  $U$ ). So if we were to apply our MinMax/Principle B to these  
 188 toy models, we would select the model corresponding to  $U_{max_{EP}}$  as the most stable one, i.e. the  
 189 conductive state with linear profile at equilibrium, and the convective state with flattened profile at  
 190 non-equilibrium. Interestingly enough, this selection corresponds qualitatively to the type of profiles  
 191 that are selected by the non-linear dynamics in the von Karman, Rayleigh-Benard or Couette system,  
 192 as illustrated in Figure 8 for the VK flow: for low levels of fluctuations (low Reynolds or impeller  
 193 with moderately bent blades) corresponding to close to equilibrium state, the most stable state is the  
 194 symmetric state, with linear angular momentum profile. At larger fluctuation rates, the most stable  
 195 state is the bifurcated state, with flat angular momentum at the center.

196 The ability of Principle B, based only on entropy i.e. *equilibrium* notions, to predict at least  
 197 qualitatively the correct behavior of scalar transport in several non-equilibrium turbulent system  
 198 is puzzling. It would be more satisfying to connect this Principle to other notions that seem more  
 199 appropriate in the case of non-equilibrium system. This is the topic of the next section.

### 200 3.3. From Maximum Entropy Production to Kolmogorov-Sinai Entropy

The physical meaning of the thermodynamic entropy production is the measure of irreversibility: the larger  $\sigma$  the more irreversible the system [34]. It is however only a *static* quantity, being unconnected to the behavior of trajectories in the phase space. In that respect, it is not in agreement with the ideas of Jaynes that non-equilibrium systems should be characterized by a probability distribution on the trajectories in phase space, instead of just the points in phase space at equilibrium. In the context of Markov chains, Jaynes' idea provides a natural generalization of equilibrium statistical mechanics [35], by considering the Kolmogorov-Sinai entropy (KSE). There are many ways to estimate the Kolmogorov-Sinai entropy associated with a Markov chain [35,36]. The most useful one in our context is the one defined as the time derivative of the Jaynes entropy. To characterize the dynamics of the system during the time interval  $[0, t]$ , one considers the possible dynamical trajectories  $\Gamma_{[0,t]}$  and the associated probabilities  $p_{\Gamma_{[0,t]}}$ . The dynamical trajectories entropy- the Jaynes entropy- reads:

$$S_{Jaynes}(t) = - \sum_{\Gamma_{[0,t]}} p_{\Gamma_{[0,t]}} \cdot \log(p_{\Gamma_{[0,t]}}) \quad (9)$$



**Figure 9.** Location of the maximum of thermodynamic entropy production  $U_{maxEP}$  (red stars) and maxim of Kolmogorov-Sinai entropy (blue stars) as a function of  $\Delta T$ . a) Case  $L=10$  ASEP (fermion). b) Case  $L=100$  ZRP (boson). The red dashed line is the second order approximation given by Eq. (8). The blue-dashed line is the first order approximation to the location of the maxima ( Eq. (12)).

For a Markov chain we find that:

$$S_{Jaynes}(t) - S_{Jaynes}(t-1) = - \sum_{(i,j)} \mu_{i_{stat}} p_{ij} \log(p_{ij}) \quad (10)$$

Thus, the Kolmogorov-Sinai Entropy for the Markov chain is:

$$h_{KS} = - \sum_{(i,j)} \mu_{i_{stat}} p_{ij} \log(p_{ij}), \quad (11)$$

201 where  $\mu_i$  is the stationary measure and  $p_{ij}$  the transition matrix.

In the case of bosonic particles (ZRP model), the KSE can be computed analytically and it admits a maximum as a function of  $U$  [33]. The value of  $U$  corresponding to this maximum can also be computed analytically, and leads to:

$$U_{max_{KS}} = \frac{\Delta T}{4M\alpha} + o(\Delta T), \quad (12)$$

202 Such first order approximation appear to be valid even far from equilibrium (see Figure 9).  
 203 Comparing with the value for the maximum of entropy production, we see that the two maxima  
 204 coincide, to first order in  $\Delta T$  and  $1/L$ : in the continuous limit, Principle B provides the same kind of  
 205 information than a third principle that we may state as:

206 *Principle C: In certain non-equilibrium systems with coexistence of several stationary state, the most*  
 207 *stable one is that of Maximum Kolmogorov-Sinai Entropy.*

208 Is this third principle any better that the principle B? In our toy models, it seems to give the same  
 209 information than the Principle B: for ZRP, we have shown analytically that the maxima of each  
 210 principle coincide to first order in  $\Delta T$  and  $1/L$ . Numerical simulation of the ASEP system suggests  
 211 that it is also true for fermionic particles: for a given value of  $\Delta T$  the difference between the two  
 212 maxima  $\Delta U_{max} = U_{maxEP} - U_{max_{KS}}$  decreases with increasing  $L$  [32]. For a fixed  $L$ , the difference

213 between the two maxima increases with  $\Delta T$ , but never exceeds a few percent at  $L = 10$  [32], see  
 214 Figure 9).

215 In turbulent system, the test of this principle is more elaborate, because the computation of  $h_{KS}$  is not  
 216 straightforward. It would however be interesting to test it in numerical simulations.

#### 217 4. From Maximum Kolmogorov-Sinai entropy to Minimum Mixing Time in Markov 218 Chains

219 Principle C is appealing because it involves a quantity clearly connected with dynamics in the phase  
 220 space, but it is still unclear why the maximization of the entropy associated with paths in the phase  
 221 space should select the most stable stationary state, if any. To make such a link, we need to somehow  
 222 connect to the relaxation towards a stationary state, i.e. the time a system takes to reach its stationary  
 223 state. In Markov chains, such a time is well defined, and is called the mixing time. Intuitively, one  
 224 may think that the smaller the mixing time, the most probable it is to observe a given stationary state.  
 225 So there should be a link between the maximum of Kolmogorov-Sinai entropy, and the Minimum  
 226 mixing time. This link has been derived in [25], for general Markov chains defined by their adjacency  
 227 matrix  $A$  and transition matrix  $P$ , defined as follows:  $A(i, j) = 1$  if and only if there is a link between  
 228 the nodes  $i$  and  $j$  and 0 otherwise.  $P = (p_{ij})$  where  $p_{ij}$  is the probability for a particle in  $i$  to hop on  
 229 the  $j$  node. Specifically, it has been shown that Kolmogorov-Sinai entropy increases with decreasing  
 230 mixing time (see Figure 1 in [25]). More generally, for a given degree of sparseness of the matrix  
 231  $A$  (number of 0), the Markov process maximizing the Kolmogorov-Sinai entropy is close (using an  
 232 appropriate distance) to the Markov process minimizing the mixing time. The degree of closeness  
 233 depends on the sparseness, and becomes very large with decreasing sparseness, i.e. for unconstrained  
 234 dynamics (Figure 3 in [25]).

235 This result provides us with a fourth principle in Markov chains:

236 *Principle D: In certain non-equilibrium systems with coexistence of several stationary states, the*  
 237 *most stable one is that of Minimum Mixing Time.*

238

239 Given what we have seen before, there are 4 general principle that select the same stationary state,  
 240 in the limit of large size and small deviations from out-of-equilibrium (see Figure 10). Among all 4,  
 241 the Principle that provides the better understanding of its application is the Principle D, because the  
 242 smaller the mixing time, the less time it is required to reach a given state and so the most probable the  
 243 corresponding state. This phenomenological understanding can actually be given a deeper meaning  
 244 when switching from Markov chains to Langevin systems.

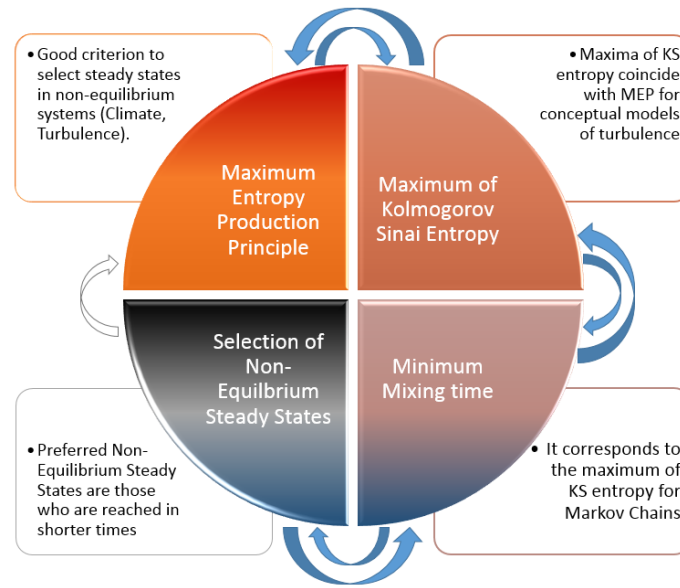
#### 245 5. From Minimum Mixing Time in Markov Chains to Mean Escape rate in Langevin 246 systems

The notions we have derived in Markov chains have actually a natural counter-part in general Langevin systems. Consider indeed the general Langevin model:

$$\dot{x} = f(x) + \zeta, \quad (13)$$

where  $f(x)$  is the force and  $\zeta$  is a delta-correlated Gaussian noise:

$$\langle \zeta \rangle = 0, \quad \langle \zeta(t)\zeta(t') \rangle = 2D\delta(t - t'). \quad (14)$$



**Figure 10.** Conceptual path to demonstrate the validity of the Maximum Entropy Principle followed in this paper.

247 The probability distribution of  $x$ ,  $P(x, t)$  then obeys a Fokker-Planck equation:

$$\begin{aligned}\partial_t P(x, t) &= -\partial_x(f(x)P(x, t)) + D\partial_x\partial_x P(x, t), \\ &= \partial_x(J(x, t)P(x, t)),\end{aligned}\quad (15)$$

where  $J = f(x)P(x, t) - D\partial_x P(x, t)$  is the current. It is well known (see e.g. [37]) that the discretization of the Langevin model on a lattice of grid spacing  $a$  (so that  $x = na$ ) is a Markov chain, governed by the master equation:

$$\partial_t P_n = w_{n-1}^+ P_{n-1} - w_n^+ P_n + w_{n+1}^- P_{n+1} - w_n^- P_n, \quad (16)$$

248 where  $P_n$  is the probability of having the particle at node  $n$  and  $w_n^\pm$  are the probability of forward and  
249 backward jump at node  $n$ , given by:

$$\begin{aligned}w_n^+ &= \frac{D}{a^2}, \\ w_n^- &= \frac{D}{a^2} - \frac{f_n}{a}.\end{aligned}\quad (17)$$

From this, we can compute the Kolomogorov-Sinai entropy as [38]

$$h_{KSL} = \langle w_n^+ \ln \frac{w_n^+}{w_{n+1}^-} + w_n^- \ln \frac{w_n^-}{w_{n-1}^+} \rangle, \quad (18)$$

which in the continuous limit  $a \rightarrow 0$  becomes:

$$h_{KSLc} = \langle \frac{1}{D} |f(x)|^2 + f'(x) \rangle, \quad (19)$$

250 which is the well know entropy production.

On the other hand, the dissipated power in the Langevin process can easily be computed as :

$$\mathcal{P} = \langle f\dot{x} \rangle = \int J(x, t)f(x, t)dx = \langle |f|^2 + Df'(x) \rangle = Dh_{KSLc}. \quad (20)$$

251 The Kolmogorov-Sinai entropy and the dissipated power are thus proportional to each other. In such  
 252 example, it is thus clear that maxima of  $h_{KS}$  and maxima of entropy production coincide.

253 On the other hand, when  $f$  derives from a potential,  $f = -\partial_x(U)$ , there may be several meta-stable  
 254 positions at  $U$  local minima. In such a case, it is known from diffusion maps theory and spectral  
 255 clustering [39] that the exit times from the meta-stable states are connected to the smallest eigenvalues  
 256 of the operator  $\mathcal{H}$ , such that  $\mathcal{H}P = D\Delta P - \nabla P \nabla U$ , which is the equivalent of the Liouville operator  
 257 in Markov chain. More specifically, if  $U$  has  $N$  local minima, then the spectra of  $\mathcal{H}$  has a cluster  
 258 of  $N$  eigenvalues  $\mu_1 < \mu_2 < \dots < \mu_N$  located near 0, each of which being associated with the exit  
 259 time it takes to get out from the local minima  $S_i$  to the state corresponding to the deepest minimum  
 260 (the equilibrium state). For example,  $\mu_1 = \frac{1}{\tau_1}$ , where  $\tau_1$  is the mean exit time to jump the highest  
 261 barrier of energy onto the deepest well. We see from that that the smaller the eigenvalue (equivalent  
 262 to the mixing time), the longer time it takes to jump from this metastable state, and so the *more*  
 263 *stable* is this state. This provides a quantitative justification of the notion that *the most stable stationary*  
 264 *states* are the one with the minimum mixing time. It is worth mentioning that Langevin systems  
 265 are now incorporated in numerical weather prediction to provide some flexibility to the sub-grid  
 266 scales parameterizations [40]. Models based on these so-called stochastic parameterizations have  
 267 usually better prediction skills than models based on deterministic parameterizations. Stochastic  
 268 parameterization is therefore increasingly used in different aspects of weather and climate modeling  
 269 [41]. We might speculate that, in these large simulations, the stochasticity helps models to reach more  
 270 realistic results by favoring jumps to *more stable* states as outlined above. Another way to select these  
 271 more realistic states could possibly be to search for the ones that maximize dissipation or entropy  
 272 production, as was done empirically in a simple way in Paltridge's model [13,14].

## 273 6. Summary: Turbulence as a minimum Mixing Time State?

274 Considering a *mixing time* to characterize turbulence is natural, given the well known enhancement  
 275 of mixing properties observed in turbulent flows. The mixing time defined for Markov chains is  
 276 also comparable to the mixing time one would naturally define for turbulence, namely the smallest  
 277 time after which a given partition of a scale quantity is uniformly spread over the volume. This time  
 278 corresponds to the one defined by Arnold for dynamical systems [42] when introducing the concept  
 279 of strong mixing. Here, it is the time associated with eigenvalues of the Liouville operator of the  
 280 processes describing the turbulence action. In the specific example we consider here, namely von  
 281 Karman flow, the turbulence is characterized by a symmetry along the rotation axis, which favors  
 282 stationary states in which angular momentum is mixed along meridional planes [43,44]. In this case,  
 283 there is a clear connection between the equation obeying the angular momentum and the classical  
 284 Fokker-Planck equation Eq. (15). One can thus hope in such a case to find a Langevin process  
 285 describing the angular momentum mixing. This was actually done in [43] and shown to reproduce  
 286 very well the power statistics in both regimes of constant torque and constant speed forcing, in case  
 287 where there is only one stationary state. For multiple stationary states, obtained in the regime with  
 288 fixed applied torque, the corresponding Langevin process has been derived in [45] and it turns out  
 289 to be a non-linear stochastic oscillator, featuring multiple metastable states and limit cycles. Such  
 290 oscillator is found to describe the dynamics of the reduced frequency  $\theta = (f_1 - f_2)/(f_1 + f_2)$  which  
 291 is a global observable respecting the symmetries of the flow. The challenge is then to compute the  
 292 mixing times of the different metastable states arising in the non-linear stochastic oscillator.

293 In [46–48] we have shown that the mixing time  $\tau$  of turbulent flows can be easily obtained by fitting  
 294 the Langevin process (or auto-regressive process)  $x_t = \phi x_{t-1} + \zeta(t)$  to data. Here  $x(t)$  is a global  
 295 quantity tracing the symmetry of the flows,  $\zeta(t)$  is a random variable normally distributed and  $-1 <$   
 296  $\phi < 1$  is the so called auto-regressive coefficient. The link with the mixing time is made through  
 297 the parameter  $|\phi|$  which is indeed proportional to  $\tau$ : the larger this quantity, the slower the mixing

298 in the system, because the dynamics weight more the present observation  $x_t$  when updating  $x_{t+1}$ .  
299 In [46], only flow configurations with a single stationary state have been analysed and  $\phi$  computed  
300 using the complete time series. To extend the results to the flow regimes featuring multistability, we  
301 use the strategy outlined in [49]. First of all, we reconstruct the dynamics by using the embedding  
302 methodology on the series of partial maxima of  $\theta$ , denoted as  $\theta_i$ . A 2D section of the attractor is  
303 shown in the upper panel of Figure 11 and it is obtained by plotting  $\theta_i$  as a function of the subsequent  
304 maxima  $\theta_{i+1}$ . The histogram of  $\theta_i$  is reported in the lower panel and show the correspondence to three  
305 metastable states  $s_1, s_2, s_3$ . Since we are not dealing with a stationary process, we cannot compute a  
306 single  $\phi$  for the full time series of  $\theta$ . The method introduced in [49] consists in computing a value of  
307  $\phi_i$  for each  $\theta_i$ , taking the 50 previous observations of the complete time series. The distribution of  $|\phi|$   
308 is shown in colorscale in Figure 11. It is evident that the most represented states ( $s_1$  and  $s_2$ ) are those  
309 with the minimum mixing time whereas the most unstable one ( $s_3$ ) is the one with the largest mixing  
310 time. This example shows that the results outlined in Section 5 can be extended to higher dimensions  
311 and that there is a simple strategy to compute the mixing times in complex systems.

312 It is quite plausible that such study can be generalized to turbulent systems with other symmetry,  
313 such as symmetry by translation along an axis. The turbulent shear flow enter in that category.  
314 Finally, we note that in Rayleigh-Bénard systems or in stratified turbulence, the temperature is also a  
315 quantity that is mixed within the flow, and that should also be liable to a Langevin description. It is  
316 therefore not a coincidence that shear flow, Rayleigh-Bénard convection and von Karman flows are  
317 so far the only systems in which the principle of Maximum Energy dissipation has been applied with  
318 some success. They are systems where a Langevin description is possible, and where the Maximum  
319 Energy dissipation principle in fact coincides with the Minimum Mixing time principle, connected  
320 to the longest exit time from meta-stable states. As observed by [50], these flows tends to be in  
321 a steady state with a distribution of eddies that produce the maximum rate of entropy increase in  
322 the nonequilibrium surroundings. In more general turbulence, it is not clear that such a Langevin  
323 description is possible, so that the statement of *Turbulence as a minimum Mixing Time State* might  
324 actually be limited to quite special situations, where symmetry or dynamics impose pure mixing  
325 of a quantity (like angular momentum, momentum or temperature). Shear flow, Rayleigh Benard  
326 convection and von Karman flows belong to this category.

327 Other conceptual pathways allow to link MEP to the underlying dynamics of the system: Moroz  
328 [51] suggests that the dissipation time minimization is linked to the least action principle, used  
329 in chemistry, biology and physics to derive the equations of motion. Although this theoretical  
330 formulation goes in the same direction of the results provided in this paper, our approach provides a  
331 rather practical way to connect dynamics and thermodynamics through statistical quantities directly  
332 computable from experimental time series.

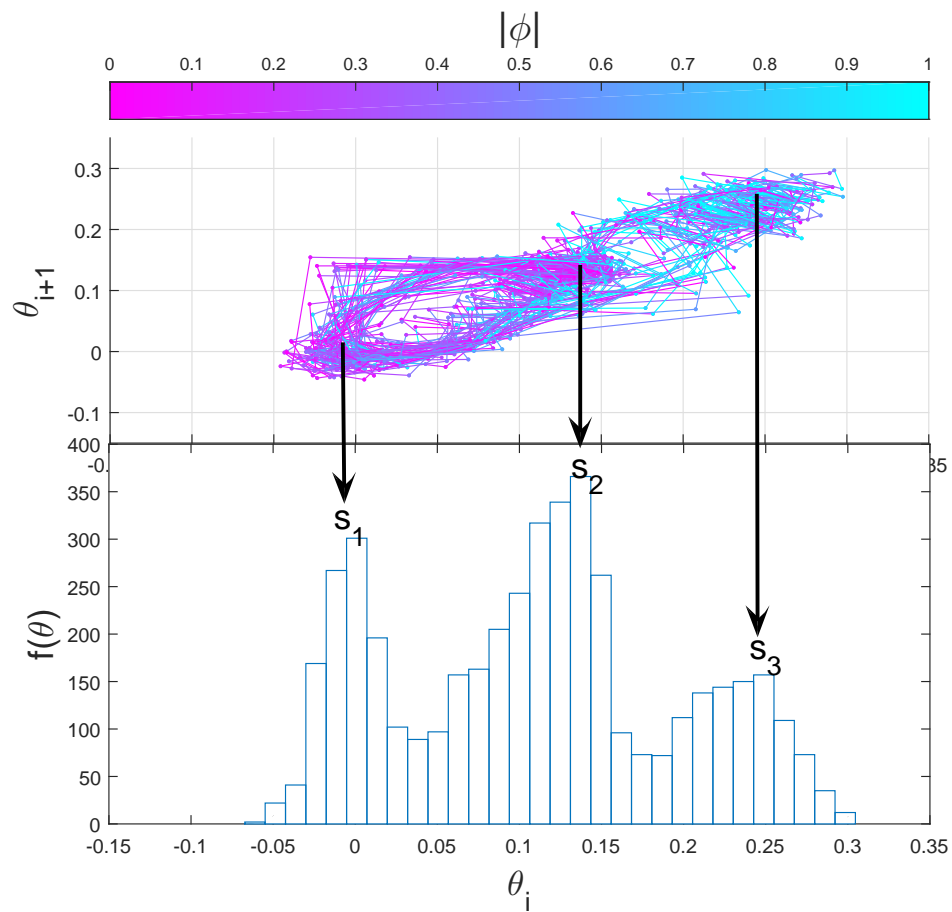
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336 the numerical computations; M.M. B.D. and D.F. analyzed the data; all the authors wrote the paper.

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**Figure 11.** Upper panel: 2D Poincaré section of the Von Karman attractor obtained embedding the partial maxima of the reduced frequency  $\theta_i$ . The colors represent  $|\phi|$ , the autoregressive coefficient computed for each of the  $\theta_i$ , using the 50 previous observations of the full time series of  $\theta$ . Lower panel: histogram of the partial maxima  $\theta_i$ . The metastable state  $s_3$  is visited less than  $s_1$  and  $s_2$  and corresponds to higher mixing time (values of  $|\phi|$  close to 1)

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