

DESCRIBING THE STATISTICS OF TURBULENT FLOW BY USING THE PRINCIPLE OF MAXIMUM ENTROPY

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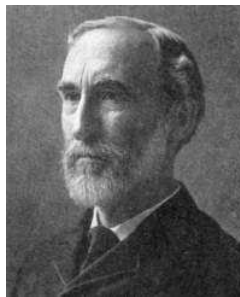
1. Turbulent flow and statistical mechanics
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1. Turbulent flow and statistical mechanics

Statistical mechanics was aimed at the description of large systems of atoms or molecules and was founded by Boltzmann (1844-1906), Maxwell (1831-1879) and Gibbs (1839-1903).

However, it also seems to be a natural framework to formulate a theory of turbulent flow.

Burgers (1895-1981) and Onsager (1903-1976) were early pioneers in applying statistical mechanics to turbulent flow.



Statistical mechanics requires a so-called *phase space*, an abstract multi-dimensional vector space defined by the degrees of freedom of the system.

For atomic or molecular systems this phase space is given by the positions q_i and momenta p_i of the particles. This phase space has $6N$ dimensions, where N is the total number of particles.

Defining a phase space of a fluid is not straightforward because a fluid is conceived of as a continuum.

Burgers proposed to describe the state of a fluid by expanding it in *basis functions*. Onsager represented it by *point vortices*.

Gibbs introduced the concept of an *ensemble*: a set of identical systems that differ in their *microscopic* properties (their position in phase space) but have the same *macroscopic* properties. In atomic or molecular systems the (conserved) total energy is the central macroscopic quantity.

In the *microcanonical ensemble* all microstates with a given energy $E(q_1, \dots, p_{3N}) = E_0$ are equally probable:

$$\mathcal{P}(q_1, \dots, p_{3N}) = \frac{\delta(E(q_1, \dots, p_{3N}) - E_0)}{\int dq_1 \cdots \int dp_{3N} \delta(E(q_1, \dots, p_{3N}) - E_0)}$$

In the *canonical ensemble* the probability of the microstates depends exponentially on the energy:

$$\mathcal{P}(q_1, \dots, p_{3N}) = \frac{\exp(-\beta E(q_1, \dots, p_{3N}))}{\int dq_1 \cdots \int dp_{3N} \exp(-\beta E(q_1, \dots, p_{3N}))}$$

The value of $\beta = \frac{1}{kT}$ is given by $\langle E \rangle = \frac{3}{2}N(1/\beta) = E_0$.

2. The maximum entropy principle

The microcanonical and canonical ensembles have the property that the *statistical mechanical entropy* defined by

$$S_T = -k \int dq_1 \cdots \int dp_{3N} \mathcal{P}(q_1, \dots, p_{3N}) \log \frac{\mathcal{P}(q_1, \dots, p_{3N})}{\mathcal{M}(q_1, \dots, p_{3N})}$$

is *maximal* among all ensembles for which $E = E_0$ and $\langle E \rangle = E_0$, respectively. (The ensemble $\mathcal{M}$ is usually just a constant.)

The statistical mechanical entropy S_T has the same mathematical form as the *information entropy* S_I which, for a general system with abstract coordinates $x_1, x_2, \dots, x_N$ and a-priori probability density function $\mathcal{M}(x_1, x_2, \dots, x_N)$, is given by:

$$S_I = - \int dx_1 \cdots \int dx_N \mathcal{P}(x_1, \dots, x_N) \log \frac{\mathcal{P}(x_1, \dots, x_N)}{\mathcal{M}(x_1, \dots, x_N)}$$

The information entropy has been introduced by Shannon (1916 - 2001) as a means of quantifying errors in the transmission of coded messages. Because of the resemblance with the statistical mechanical entropy von Neumann (1903-1957) has suggested to give it a similar name.

Jaynes (1922 - 1988) raised the observation that the basic ensembles of statistical mechanics maximize the statistical mechanical entropy to a *general principle*: any probability density function that quantifies an uncertain state, in a way that is as non-committal as possible, should have maximal information entropy.



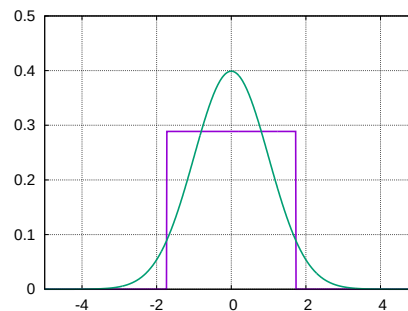
A nice example of maximum entropy is the normal distribution:

$$\mathcal{N}(\mu, \sigma, x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

with mean $\langle x \rangle = \mu$ and variance $\langle (x - \langle x \rangle)^2 \rangle = \sigma^2$. The information entropy (c is arbitrary) is:

$$S_I = - \int_{-\infty}^{+\infty} dx \mathcal{P}(x) \log \frac{\mathcal{P}(x)}{1/c} = 1/2 \log[2\pi e(\sigma/c)^2]$$

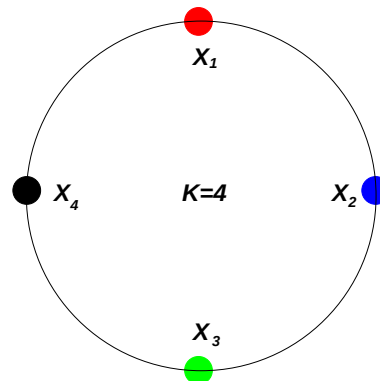
No distribution with the same mean μ and variance σ^2 has a higher entropy. E.g. a hat-like probability density function with the same mean and variance has the lower value $1/2 \log[12(\sigma/c)^2]$.



3. The system of Lorenz (1996)*

Lorenz (1996) devised a model for the purpose of atmospheric predictability studies. It reads:

$$\frac{dX_k}{dt} = X_{k-1}(X_{k+1} - X_{k-2}) - X_k + F, \quad k = 1, \dots, K.$$



The variables are cyclic in the sense that $X_{k-K} = X_{k+K} = X_k$. In the following we use $K = 36$.

*Verkley and Severijns (EPJB, 2014)

The energy of Lorenz' system is simply:

$$E = \sum_{k=1}^K \frac{1}{2} X_k^2$$

For the first-order and second-order time-derivatives of the energy we have:

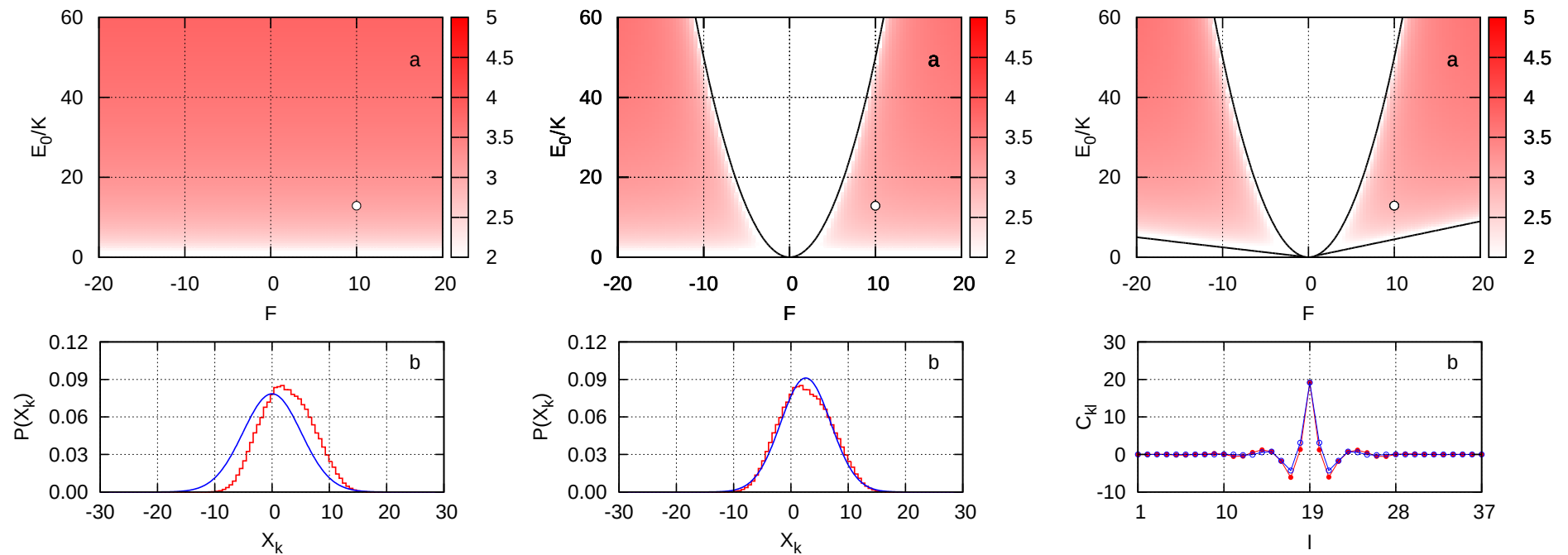
$$\frac{dE}{dt} = -2E + F \sum_{k=1}^K X_k$$

$$\frac{d^2 E}{dt^2} = -2 \frac{dE}{dt} + F \sum_{k=1}^K (F + X_k(X_{k+2} - X_{k+1} - 1))$$

We search for probability density functions $\mathcal{P}(X_1, \dots, X_k)$ that have maximal information entropy under several combinations of constraints: $\langle E \rangle = E_0$, $\langle dE/dt \rangle = 0$ and $\langle d^2 E/dt^2 \rangle = 0$.

Results

The upper graphs show the maximum entropy S_M/K as a function of the forcing F and the energy E_0/K . The lower graphs show the numerical (red) and analytical (blue) marginal probability density functions (left and middle) and covariances (right).



4. The vorticity equation*

The basic evolution equation is the advection of vorticity ζ :

$$\frac{\partial \zeta}{\partial t} + J(\psi, \zeta) = \nu \nabla^8 \zeta + \mu(F - \zeta)$$

Here ψ is the streamfunction of the velocity field $\mathbf{v}$. The domain S is a doubly periodic square of size 2π . We use a numerical model in which ζ (and ψ) are written as:

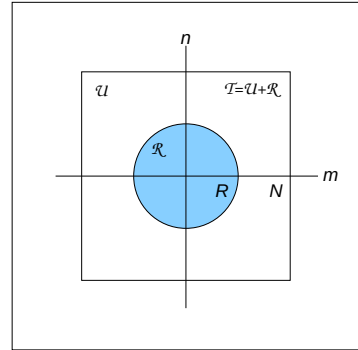
$$\zeta(x, y, t) = \sum_{(m,n) \in \mathcal{T}} \zeta_{mn}(t) Y_{mn}(x, y)$$

where $Y_{mn} = X_m(x)X_n(y)$ with $X_m(x)$ and $X_n(y)$ sines and cosines with argument mx and ny , respectively.

*Verkley, Kalverla, Severijns (QJRMS, 2014), Verkley, Severijns, Zwaal (QJRMS, 2019)

In order to distinguish between *resolved* and *unresolved* scales in the context of this idealized set-up, we write $\zeta = \zeta^{\mathcal{R}} + \zeta^{\mathcal{U}}$ with:

$$\zeta^{\mathcal{R}} = \sum_{(m,n) \in \mathcal{R}} \zeta_{mn} Y_{mn} \quad \zeta^{\mathcal{U}} = \sum_{(m,n) \in \mathcal{U}} \zeta_{mn} Y_{mn}$$



The original vorticity equation can be written as:

$$\begin{aligned} \frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}} + \psi^{\mathcal{U}}, \zeta^{\mathcal{R}} + \zeta^{\mathcal{U}}) &= \nu \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}}) \\ \frac{\partial \zeta^{\mathcal{U}}}{\partial t} + P^{\mathcal{U}} J(\psi^{\mathcal{R}} + \psi^{\mathcal{U}}, \zeta^{\mathcal{R}} + \zeta^{\mathcal{U}}) &= \nu \nabla^8 \zeta^{\mathcal{U}} + \mu(F^{\mathcal{U}} - \zeta^{\mathcal{U}}) \end{aligned}$$

The equation for the resolved scales reads:

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}} + \psi^{\mathcal{U}}, \zeta^{\mathcal{R}} + \zeta^{\mathcal{U}}) = \nu \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}})$$

The simplest parameterization is to skip the unresolved scales:

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}} + 0, \zeta^{\mathcal{R}} + 0) = \nu \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}})$$

The second option (eddy hyperviscosity) is to increase ν to ν' :

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}}, \zeta^{\mathcal{R}}) = \nu' \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}})$$

A third option is to use a probability density function for the unresolved scales and average over this probability density function:

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} \langle J(\psi^{\mathcal{R}} + \psi^{\mathcal{U}}, \zeta^{\mathcal{R}} + \zeta^{\mathcal{U}}) \rangle = \nu \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}})$$

The probability density function follows from *maximum entropy*.

The energy and enstrophy of the unresolved scales is:

$$E^{\mathcal{U}} = \sum_{(m,n) \in \mathcal{U}} \frac{1}{2} \frac{\zeta_{mn}^2}{c_{mn}} \quad Z^{\mathcal{U}} = \sum_{(m,n) \in \mathcal{U}} \frac{1}{2} \zeta_{mn}^2$$

The unresolved scales' energy and enstrophy change in time:

$$\begin{aligned} \frac{dE^{\mathcal{U}}}{dt} = & -\nu \sum_{(m,n) \in \mathcal{U}} c_{mn}^3 \zeta_{mn}^2 + \mu \sum_{(m,n) \in \mathcal{U}} \frac{1}{c_{mn}} (F_{mn} - \zeta_{mn}) \zeta_{mn} \\ & - \sum_{(m,n) \in \mathcal{U}} \frac{1}{c_{mn}} (Y_{mn}, J(\psi^{\mathcal{R}}, \zeta^{\mathcal{R}})) \zeta_{mn} + \dots \end{aligned}$$

$$\begin{aligned} \frac{dZ^{\mathcal{U}}}{dt} = & -\nu \sum_{(m,n) \in \mathcal{U}} c_{mn}^4 \zeta_{mn}^2 + \mu \sum_{(m,n) \in \mathcal{U}} (F_{mn} - \zeta_{mn}) \zeta_{mn} \\ & - \sum_{(m,n) \in \mathcal{U}} (Y_{mn}, J(\psi^{\mathcal{R}}, \zeta^{\mathcal{R}})) \zeta_{mn} + \dots \end{aligned}$$

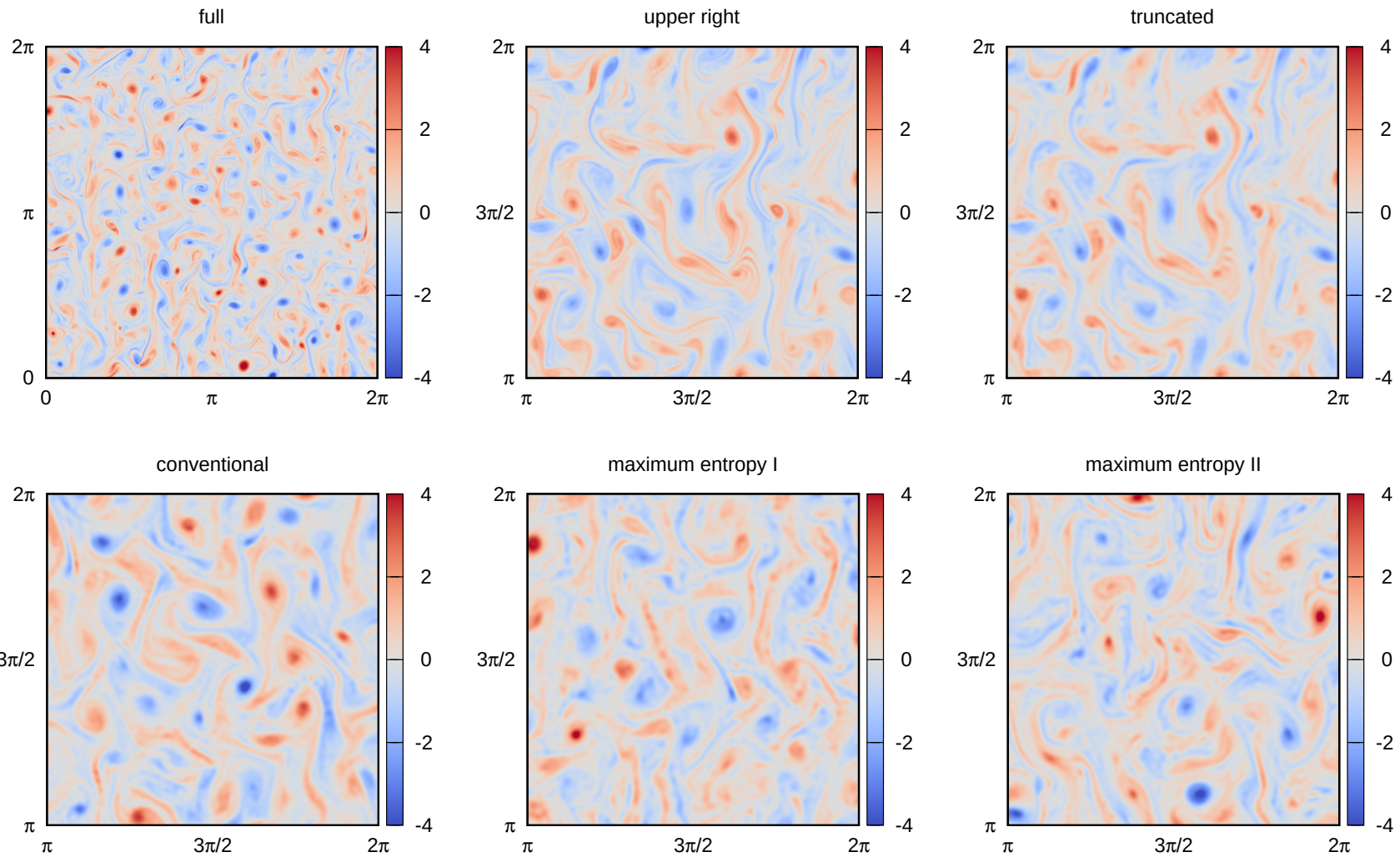
The probability density function of the unresolved scales, denoted by $\mathcal{P}(\zeta^U)$, is obtained by maximizing the information entropy under different combinations of constraints:

$$\begin{aligned} \text{I} \quad & \left\langle \frac{dE^U}{dt} \right\rangle = 0, \quad \left\langle \frac{dZ^U}{dt} \right\rangle = 0 \\ \text{II} \quad & \left\langle \frac{dE^U}{dt} \right\rangle = 0, \quad \langle E^U \rangle = E_0^U \end{aligned}$$

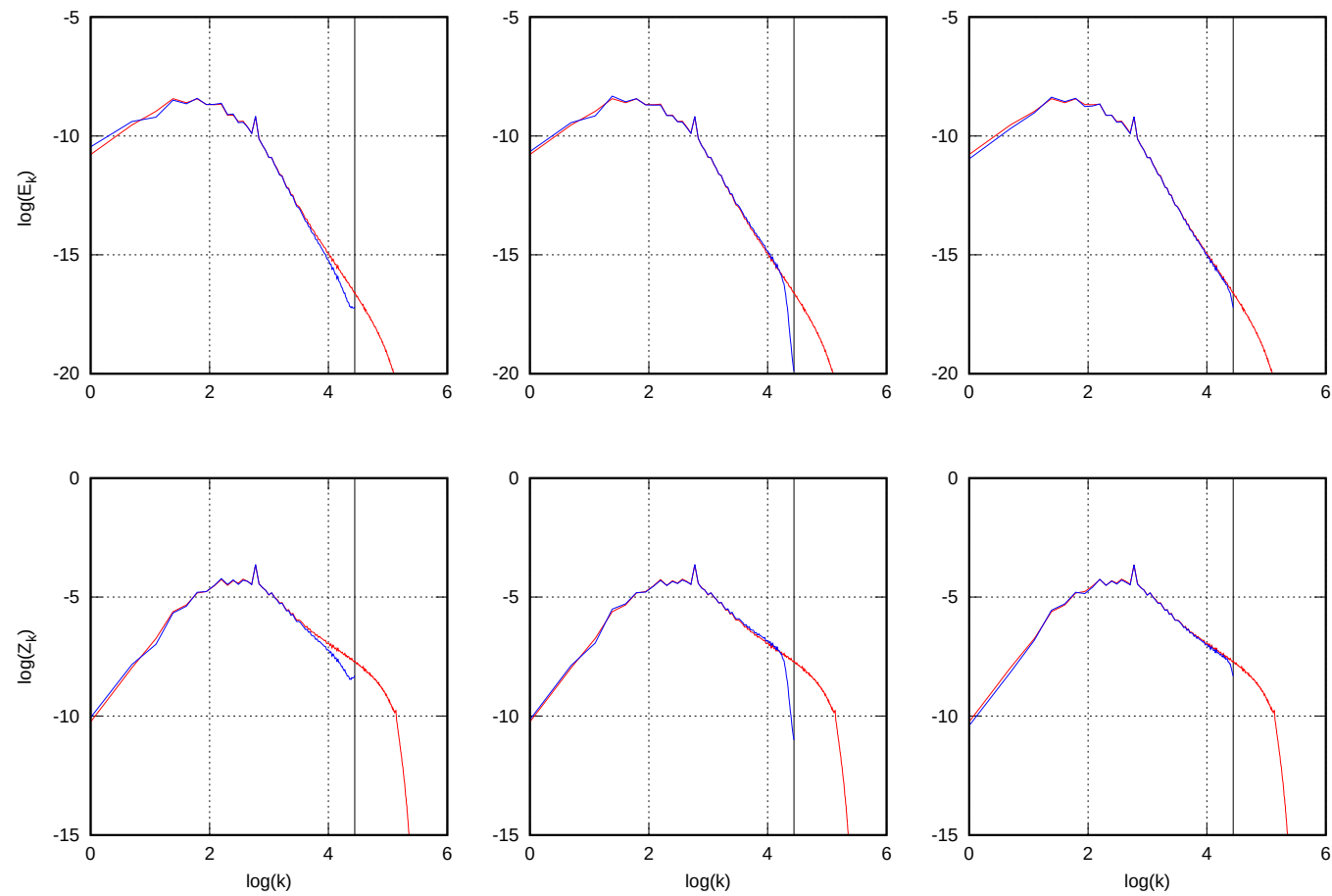
On the basis of the resulting probability density function one can calculate $\langle \psi^U \rangle$ and $\langle \zeta^U \rangle$. Due to our approximation $\langle J(\psi^U, \zeta^U) \rangle = J(\langle \psi^U \rangle, \langle \zeta^U \rangle)$ and we find for the resolved scales:

$$\frac{\partial \zeta^{\mathcal{R}}}{\partial t} + P^{\mathcal{R}} J(\psi^{\mathcal{R}} + \langle \psi^U \rangle, \zeta^{\mathcal{R}} + \langle \zeta^U \rangle) = \nu \nabla^8 \zeta^{\mathcal{R}} + \mu(F^{\mathcal{R}} - \zeta^{\mathcal{R}})$$

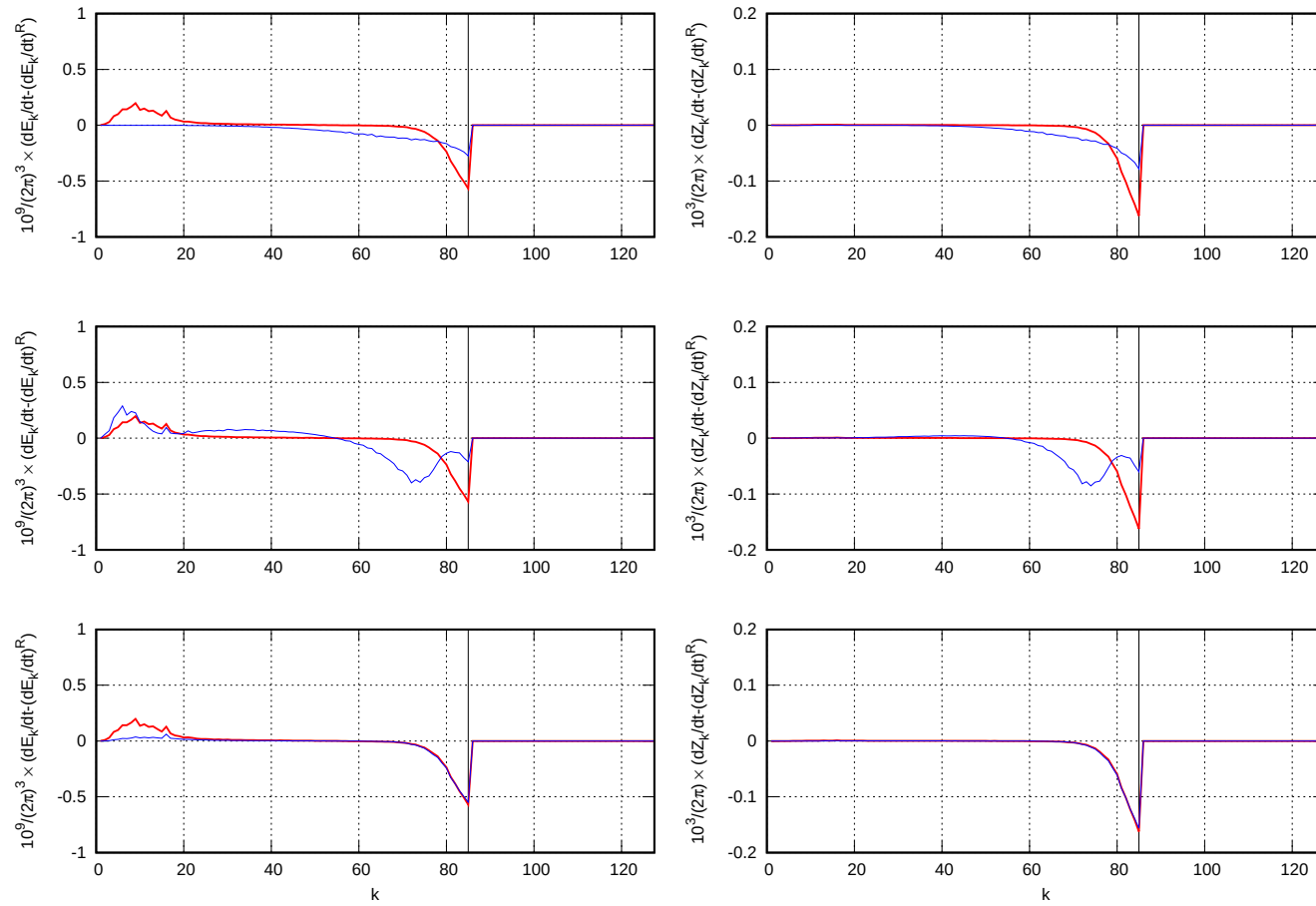
Vorticity fields:



Spectra of energy and enstrophy:



Spectral transfer of energy and enstrophy:



5. Summary

The information entropy, introduced by Shannon to quantify errors in the transmission of coded messages, has the same mathematical form as the statistical mechanical entropy.

The ensembles of equilibrium statistical mechanics have the property that they maximize the information entropy. Jaynes has promoted this observation to a general principle.

The principle is: probability density functions that are meant to describe an uncertain state of affairs in a way that is as noncommittal as possible should have maximal information entropy.

The maximization of entropy is subject to constraints. These constraints, including the normalization constraint, determine the form of the maximum entropy probability density function.

Formulated in this general form the principle of maximum entropy can be applied to many systems, in particular to forced-dissipative systems such as turbulence.

In these forced-dissipative systems the balance between forcing and dissipation of energy is an important constraint that can be dealt with in much the same way as the energy itself.

For the statistics of turbulence (more generally, chaotic dynamics) and the parametrization of unresolved scales, the principle of maximum entropy was seen to give sensible results.

Mathematical questions: how do you deal with infinite-dimensional phase spaces and constraints that are more complicated than quadratic? Physical question: what are the relevant constraints?