The statistical mechanics of turbulent flows

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Introduction

In a paper that appeared 70 years ago in the Journal of the Dutch Physical Society, Burgers[1] addressed the question whether the statistics of turbulent flows can be investigated by the methods of statistical mechanics.

In the past these methods had been very successfully applied to the microscopic motion of molecules. In extending their application to the realm of turbulent motion, one encounters the difficulty that the fluid dynamical equations are continuous. By using a representation of the flow fields in terms of Fourier components this problem can be solved to the extent that a phase space can still be defined although it is infinite dimensional. Another difficulty is that, in turbulent motion, energy is not conserved but flows through the system. Burgers therefore proposed that the statistics of a turbulent system is controlled by an average balance between input and output of energy and not, as is appropriate to assume in the realm of molecular motion, by the conservation of energy. Taking the dissipation to be quadratic, when expressed in terms of the Fourier coefficients, and constraining the statistics to respect an average balance between forcing and dissipation, he applied the techniques of statistical mechanics and concluded that the dissipation is equally partitioned among the Fourier components.

Our aim is to deduce the model's climate from its basic equations, as an alternative to averaging over long numerical time-integrations

This conclusion was both interesting and problematic. Equipartition of dissipation leads to an unphysical infinite total dissipation if the phase space of the system is infinite dimensional. Quantum mechanics does not come to the rescue here as it had done earlier when an analogous problem arose in the statistical mechanics of electromagnetic radiation. Despite a series of publications, many of which are reprinted in the memorial volume by Nieuwstadt and Steketee[2], a completely satisfying solution did not emerge and Burgers finally abandoned the subject. Several years later Onsager[3] took it up again but decided to pursue a course that is more in line with equilibrium statistical mechanics, as detailed in the review article by Eyink and Sreenivasan[4].

The work described below[5] can be considered as an attempt to revisit Burgers' approach. It will thus be investigated whether statistical mechanics can be used to deal with forced-dissipative turbulent systems, using as a basic assumption that the statistics is controlled by an average balance between forcing and dissipation.
The problem of the infinite dissipation is not resolved but moderated by limiting ourselves to finitely truncated spectral representations of fluid flows. We will phrase the theory in the language of probability theory and the principle of maximum entropy, as advocated by Jaynes[6].

The method will be applied to a simple one-layer model of the large-scale atmospheric circulation. In this context the model's statistics can be identified with the model's climate. From the perspective of this model our aim is to deduce the model's climate from its basic equations, as an alternative to averaging over long numerical time-integrations.

A model of the large-scale atmospheric circulation

The model to be considered describes the motion of a single layer of incompressible fluid on the surface of a rotating sphere. Orography is taken into account and the flow is assumed to be geostrophically balanced and thus approximately governed by the horizontal advection of quasigeostrophic potential vorticity. The equation that is used is a somewhat simplified version of an equation discussed recently by the author[7)]. The system is forced by relaxation towards a zonally symmetric circulation that consists of jet-streams in both hemispheres, and is damped by a term that has the same structure as the viscosity term in fluid dynamics. The two-dimensional streamfunction, in terms of which the horizontal velocity is expressed, is the basic field of the model and is represented by a finite set of spherical harmonics, indexed by the integers m and n, where n runs from 1 to $N = 42$ and m runs from $-n$ to $+n$. The variables of the model are expressed in units formed by appropriate combinations of the earth's radius and angular velocity of rotation.

The phase space of the model consists of the Fourier coefficients ψ_{mn} of the streamfunction. By projecting the advection equation of potential vorticity onto the finite set of spherical harmonics, one obtains a dynamical system of quadratically non-linear equations in the Fourier coefficients. When integrated numerically, this finite-dimensional dynamical system displays chaotic turbulent motion, not unlike what is seen in large-scale atmospheric flow. To demonstrate this, we show in Figure 1 two snapshots of the vorticity and the zonally averaged zonal velocity, separated by 10 days in time, at the end of an integration of 2000 days.

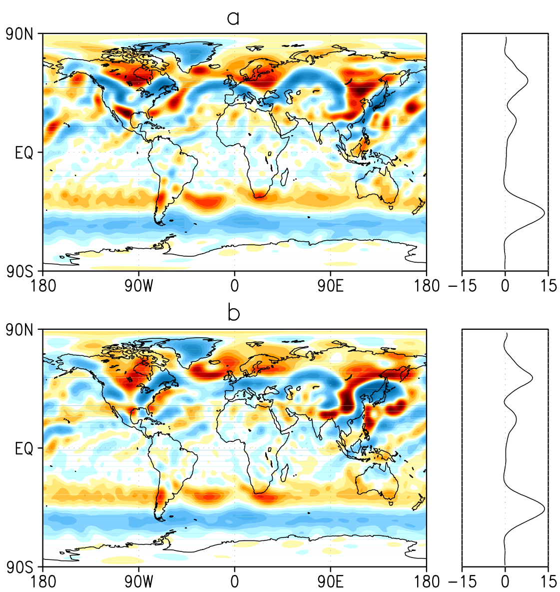

Figure 1. *The vorticity field at day 1990 and day 2000 (a and b, respectively) in a numerical integration of the spectral model of large-scale atmospheric flow. The values of the vorticity are expressed in units of the earth's angular velocity and are in the range (-0.50, 0.55) and (-0.57, 0.61), respectively, and are displayed with a contour interval of 0.04. The colour scale is from blue (low values) to red (high values). The profiles to the right of the vorticity fields are the zonally averaged zonal velocity in meters per second.*

Energy and enstrophy

The global state of the system can be characterized by the energy E and the enstrophy Z, given by

$$E = \Sigma_{mn} (1/2)\, \varepsilon_n \psi^2_{mn},$$
$$Z = \Sigma_{mn} (1/2)\, (\varepsilon_n \psi_{mn} - f_{mn})^2.$$

Here is ε_n a system parameter and f_{mn} is related to the Coriolis parameter and the orography. In the presence of forcing and dissipation, we have

$$dE/dt = F - D,$$
$$dZ/dt = G - H,$$

in which the energy forcing F, energy dissipation D, enstrophy forcing G and enstrophy dissipation H are given by

$$F = \Sigma_{mn} (-F_{mn} \psi_{mn}),$$
$$D = \Sigma_{mn} (d_n \psi^2_{mn}),$$
$$G = \Sigma_{mn} (-\varepsilon_n F_{mn} \psi_{mn} + f_{mn} F_{mn}),$$
$$H = \Sigma_{mn} (d_n \varepsilon_n \psi^2_{mn} - d_n f_{mn} \psi_{mn}).$$

In these expressions F_{mn} is the Fourier coefficient of the forcing and d_n is related to the form and the strength of the dissipation. It can be seen that, if the forcing coefficients F_{mn} and dissipation parameters d_n are zero, the energy E and the enstrophy Z are conserved. If these coefficients and parameters are not zero, this is no longer the case. However, for a statistically stationary state we have instead that dE/dt and dZ/dt, or $F - D$ and $G - H$, are zero on average.

Statistical mechanics and maximum entropy

The central concept in a statistical mechanical theory is the probability density function, denoted by P, which in our case gives the probability to find the system in a state with Fourier coefficients ψ_{mn}. According to Jaynes' principle of maximum entropy, the probability density function should have a maximum value of its information entropy S_1, defined by

$$S_I = -\int \ldots \int d\psi_{-N-N} \ldots d\psi_{NN} \times$$
$$P(\psi_{-N-N},\ldots,\psi_{NN}) \log \frac{P(\psi_{-N-N},\ldots,\psi_{NN})}{M(\psi_{-N-N},\ldots,\psi_{NN})} .$$

The measure M, for which a product of constants is taken, incorporates any a-priori knowledge of the system such as its basic symmetries. All additional information on the system is used to constrain the maximization of S_I, like the normalization condition on P. The additional information consists of fixed averages of certain functions Q, with the average $\langle Q \rangle$ defined by

$$\langle Q \rangle = \int \ldots \int d\psi_{-N-N} \ldots d\psi_{NN} \times$$
$$P(\psi_{-N-N},\ldots,\psi_{NN}) Q(\psi_{-N-N},\ldots,\psi_{NN}).$$

Without these averages as constraints, the maximization of the information entropy S_I would result in $P = M$. Although the constant values that we take to define M turn out to influence the maximum value of the information entropy S_I, these values do not influence the probability density function P and thus do not influence the resulting statistics.

In the equilibrium statistical mechanical theory that emerged from Onsager's approach, the information entropy is maximized with fixed values of the average energy $\langle E \rangle$ and the average enstrophy $\langle Z \rangle$. This has been shown[5)] to work rather well if the statistics is controlled by conservation of energy and enstrophy, i.e., in the unforced-undamped case - which is not very realistic. If forcing and dissipation are present then, in line with Burgers' approach, it is more appropriate to maximize the information entropy with fixed (zero) values of $\langle F - D \rangle$ and $\langle G - H \rangle$. Fortunately, the mathematics is similar in both cases because all constraints are quadratic and lead to a probability density function that is a product of normal distributions. Once the probability density function is known, all relevant statistics can be calculated, such as spectra of energy and enstrophy and average vorticity fields.

Results

We will focus on the numerical integration of 2000 days of which two snapshots of vorticity have been shown in Figure 1. We use the last 500 days of the integration to calculate average spectra, vorticity and velocity fields in order to compare these with the theoretical results. To define the spectra of energy and enstrophy, we write the energy E and the entrophy Z as a sum over N functions E_n and Z_n, the latter containing the sums over m. The spectra of energy and enstrophy are thus E_n and Z_n as functions of n, where n runs from 1 to 42.

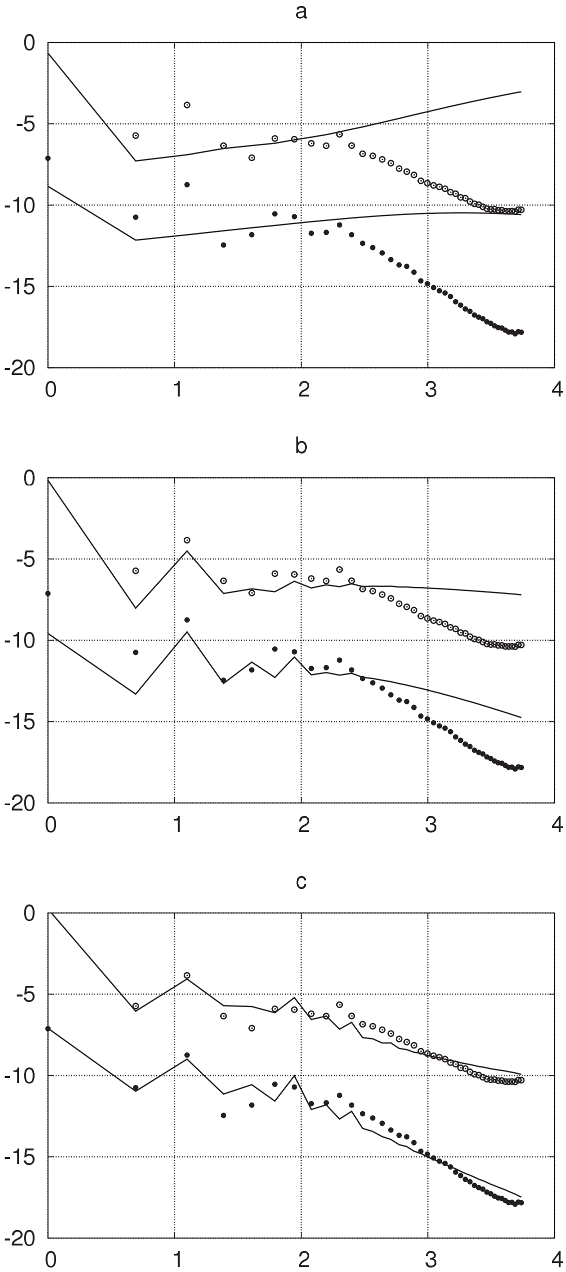

Figure 2. *The values of log E_n (energy) and log Z_n (enstrophy) as a function of log n, averaged over the last 500 days of the numerical integration. The solid dots represent the spectra of energy, the open circles represent the spectra of enstrophy and the solid curves are the theoretical spectra, based on maximum entropy. In the upper panel (a) the constraints in the maximization of entropy are energy and enstrophy, in the middle panel (b) the constraints are the decay rates of energy and enstrophy (taken to be zero), and in the lower panel (c) both energy and enstrophy as well as their decay rates are used as constraints.*

The solid dots and open circles in the three panels of Figure 2 are the numerically obtained values of log E_n and log Z_n, respectively, as a function of log n,

for $n = 1, \ldots, 42$. The solid curves in panel a are the spectra based on maximum entropy if the numerically obtained values of $\langle E \rangle$ and $\langle Z \rangle$ are used as constraints.
Whereas this has been shown to work quite well in the unforced-undamped case, in the forced-damped case that we consider here it does not work at all. The numerically obtained spectra are very different from the spectra that characterize the unforced-undamped case.

The solid lines in panel b of Figure 2 show the theoretical spectra if the entropy is maximized using as constraints that $\langle F - D \rangle$ and $\langle G - H \rangle$ are zero. This is the case that corresponds to Burgers' basic idea. In contrast to the case displayed in panel a of Figure 2, we do not need any information from the numerical run except for the fact that it has reached a state of statistical equilibrium. The resemblance between the theoretical and numerical spectra is nevertheless substantially better that in the case of panel a of Figure 2, in particular for the lower values of the wavenumber n.

In panel c of Figure 2 we show the theoretical spectra if the numerically obtained values of $\langle E \rangle$ and $\langle Z \rangle$ are used as constraints in addition to the constraints that $\langle F - D \rangle$ and $\langle G - H \rangle$ are zero. Whereas on their own the former constraints do not lead to proper spectra (as we have just seen), when combined with the constraints that $\langle F - D \rangle$ and $\langle G - H \rangle$ are zero, they lead to an improvement that is quite substantial. It shows that the values of $\langle E \rangle$ and $\langle Z \rangle$ contain useful extra information and that the theory is able to incorporate that extra information in a consistent way.
In panel a of Figure 3 we show the vorticity and zonally averaged zonal velocity obtained numerically, averaged over the last 500 days of the integration. In panel b the theoretical average is given, calculated on the basis of maximum entropy using the numerically obtained values of $\langle E \rangle$ and $\langle Z \rangle$ as constraints. In panel c the theoretical average is shown that results if zero values of $\langle F - D \rangle$ and $\langle G - H \rangle$ are used as constraints in the maximization of entropy. In panel d, finally, the result is shown if the numerically obtained values of $\langle E \rangle$ and $\langle Z \rangle$ are used as extra constraints in the maximization of entropy. The most striking difference is between panels b and c, the former showing no trace of the two jet-streams, the latter showing these jet-streams quite clearly. Panel d confirms that additional information in the form of given values of $\langle E \rangle$ and $\langle Z \rangle$ leads to theoretical results that are more in accord with the numerical simulations.

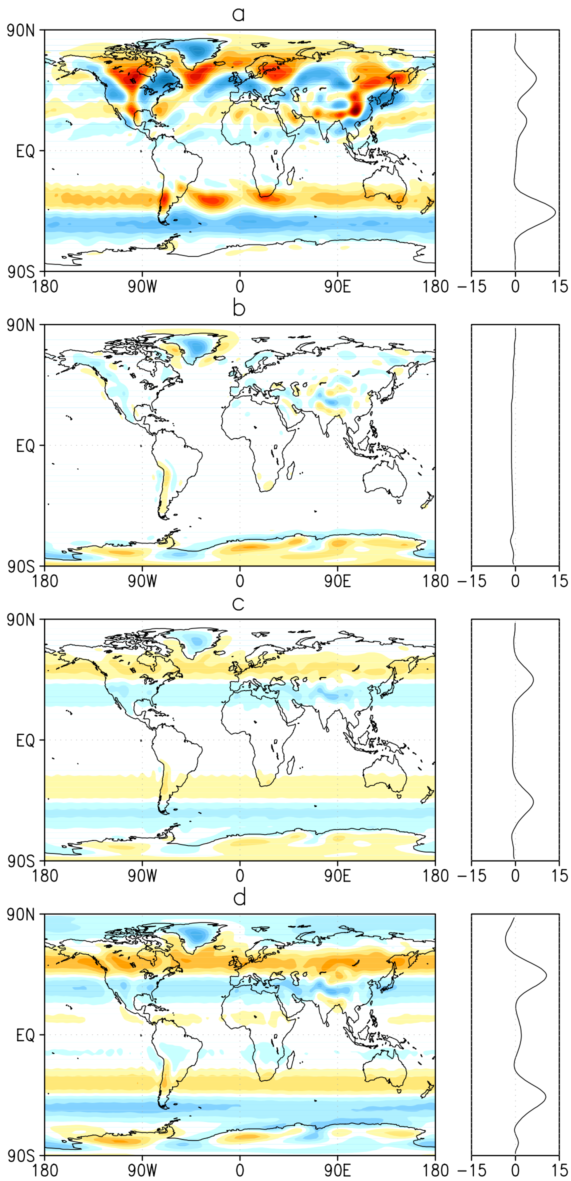

Figure 3. *Vorticity fields, expressed in units of the earth's angular velocity, displayed with a contour interval of 0.04, using the same colour scale as in Figure 1. Zonally averaged zonal velocity profiles in meters per second are displayed to the right of the vorticity fields. Panel a shows the results averaged over the last 500 days of the numerical integration. Panels b, c and d show the theoretical averages, based on maximization of entropy. The constraints in b are energy and enstrophy, in c the (zero) decay rates of energy and enstrophy and in d both energy and enstrophy and their zero decay rates. The vorticity fields in the consecutive panels vary between (-0.41, 0.46), (-0.21, 0.15), (-0.13, 0.09) and (-0.21, 0.17), respectively.*

Conclusion

We have shown that the formalism of statistical mechanics, expressed in the language of probability theory and the principle of maximum entropy, is able to produce statistics of forced-dissipative turbulent flows. The basic idea is that the statistics of a stationary turbulent system is controlled by the average balance between forcing and dissipation, an idea pursued earlier by Burgers. The theory was applied to a finitely truncated spectral model of large-scale atmospheric flow with the aim of deducing the climate of the model from its equations as an alternative to averaging over long numerical time-integrations.

The theory has shown its most predictive side if, in line with Burgers' idea, the average time derivative of energy and enstrophy are constrained to be zero in the maximization of entropy. In this case no information from the numerical run is needed except the fact that the system is in a statistically stationary state. The results compare favourably with the results obtained in the case that the energy and enstrophy, obtained from the numerical run, are used as constraints in the maximization of entropy. When all constraints are combined, the theoretical results compare best with their numerical counterparts. From the latter it may be concluded that, if the values of energy and enstrophy are available, the additional information that these values contain can be incorporated consistently by the principle of the maximum entropy.

A procedure that would avoid the use of average values of the energy and enstrophy, to be taken from the numerical run and therefore at the expense of the theory's predictive power, is to use as additional constraints the condition that the second- and higher-order time derivatives of energy and enstrophy are zero. This is justified in case the system is statistically stationary and, in view of the form of these constraints, is expected to lead to more structure in the resulting statistics such as correlations between the spectral coefficients. The price to be paid is a mathematically more complex analysis but, in view of the possibilities that it promises, would be worthwhile to pursue as a topic of further research.

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