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Control and instanton trajectories for random transitions in turbulent flows

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Abstract. Many turbulent systems exhibit random switches between qualitatively different attractors. The transition between these bistable states is often an extremely rare event, that can not be computed through DNS, due to complexity limitations. We present results for the calculation of instanton trajectories (a control problem) between non-equilibrium stationary states (attractors) in the 2D stochastic Navier-Stokes equations. By representing the transition probability between two states using a path integral formulation, we can compute the most probable trajectory (instanton) joining two non-equilibrium stationary states. Technically, this is equivalent to the minimization of an action, which can be related to a fluid mechanics control problem.

1. Introduction

Many turbulent flows undergo sporadic random transitions after long periods of very apparent statistical stationarity. For instance, the Earth's magnetic field reversal or in MHD experiments (see Fig. 1) (Berhanu *et al.*, 2007), 2D turbulence experiments (Sommeria, 1986; Maassen *et al.*, 2003), 3D flows (Ravelet *et al.*, 2004), atmospheric flows (Weeks *et al.*, 1997), and for paths of ocean currents (Schmeits & Dijkstra, 2001). This phenomena is far from understood due to the complexity, the large number of degrees of freedom, and the non-equilibrium nature of many of these flows.

A straightforward numerical approach in considering these transition events would be to simply perform a DNS of the governing equations and wait until a transition (instanton) trajectory is observed. Most of the time, this is impracticable due to the extremely long time between two transitions, very high Reynolds number and to the large number of degrees of freedom involved. We will present an alternative strategy, in which we apply instanton theory (Freidlin & Wentzell, 1998) to predict the most likely instanton trajectory between two non-equilibrium stationary states utilizing a path integral formulation (Feynman & Hibbs, 1965) in a small noise limit - a procedure that has been applied in various fields of physics (Berkov, 1998; E *et al.*, 2004).

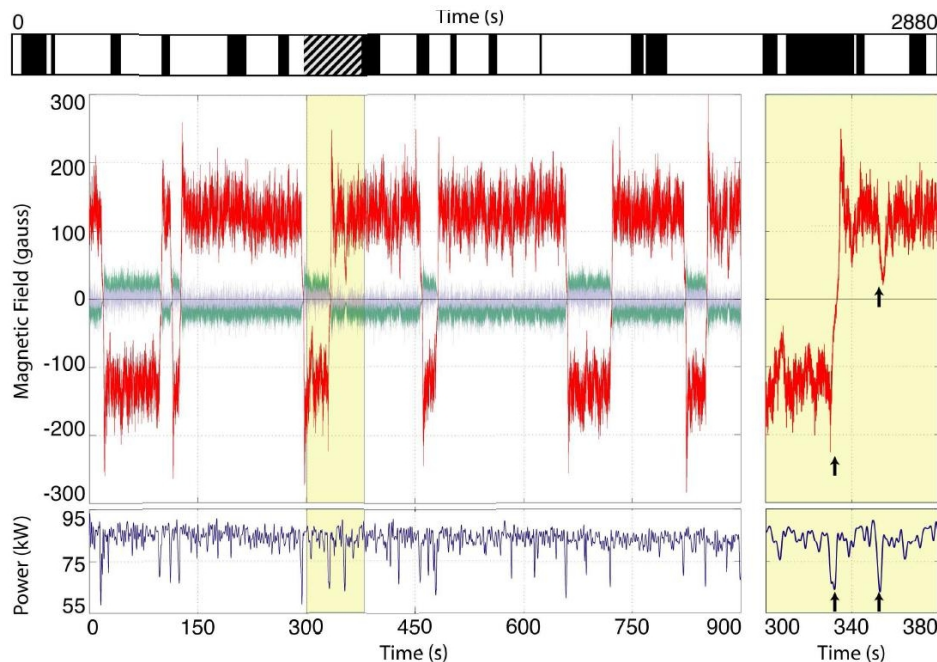


Figure 1. Figure taken from Berhanu *et al.* (2007) showing random transitions between orientations of a magnetic field in an experimental dynamo. The main azimuthal component of the magnetic field is shown in red. The top graphic shows the magnetic field orientation, white for a positive direction, black for the negative direction. The bottom graph shows synchronous recordings of the power driving the flow.

2. Control and instanton theory

The transition probability is the probability of the system starting from a state A, to reach a state B after a time interval T . It is thus an essential dynamical quantity that encodes most of statistics of the system. For bistable systems with weak noise, the transition from one attractor to the other is an extremely rare event. However, as paradoxical as it may seem, most of the trajectories joining the two states are concentrated close to a single one: the instanton trajectory.

Instanton theory is a way of determining this most probable transition trajectory between two states in a non-equilibrium dynamical system with small noise, using a path integral formulation. The transition probability is then represented using the Onsager-Machlup path integral over all possible paths between the two states:

$$P(\omega, t; \omega(0) = \omega_0, \omega(T) = \omega_T) = \int \mathcal{D}[\omega] e^{-\frac{1}{4\sigma} S(\omega)}.$$

Here, deviation from the deterministic (zero noise) trajectory is represented by a ‘cost’ function that exponentially diminishes the probability the further away from the deterministic trajectory one gets. The exponent of the exponential is proportional to the inverse of the noise amplitude σ and some specific action $S(x)$ for the system. Instanton theory uses the saddle point method in the limit of small amplitude noise ($\sigma \rightarrow 0$) to show that the most probable transition trajectory (and henceforth the maximizer of the exponential) is the trajectory that minimizes the action $S(\omega)$ - this trajectory ω^* is what is known as the instanton. Therefore, the main contribution to the transition probability arises from the value of the action on the instanton trajectory:

$$P(\omega, t; \omega(0) = \omega_0, \omega(T) = \omega_T) \approx e^{-\frac{1}{4\sigma} S(\omega^*)}. \quad (1)$$

Eq. (1) is also known as a large deviation principle (Freidlin & Wentzell, 1998; Touchette, 2009).

The transition probability for the instanton can then be used to estimate the timescale of observing such a trajectory. Because of the large separation of timescales, usually it is far more efficient to compute the minimizer of an action than to perform a DNS of the system until a transition trajectory is observed.

3. Application to the 2D Navier-Stokes equations

We apply the formalism of instanton theory to the 2D Navier-Stokes equations with stochastic forcing - a new approach to this type of phenomena. We show that by minimizing an appropriate action, we can predict the most probable instanton trajectory between two non-equilibrium stationary states.

We consider the 2D stochastic Navier-Stokes equations in a regime of small forcing and dissipation. In this case, the largest scales of the flow self-organize to produce coherent jets and vortices. Moreover it was recently shown that over long times, random switches between two non-equilibrium stationary states can occur - more precisely between a parallel and dipole flow (Bouchet & Simonnet, 2009) (see Fig. 2). It is this behavior that has given us the motivation to apply instanton theory to the 2D stochastic Navier-Stokes equations.

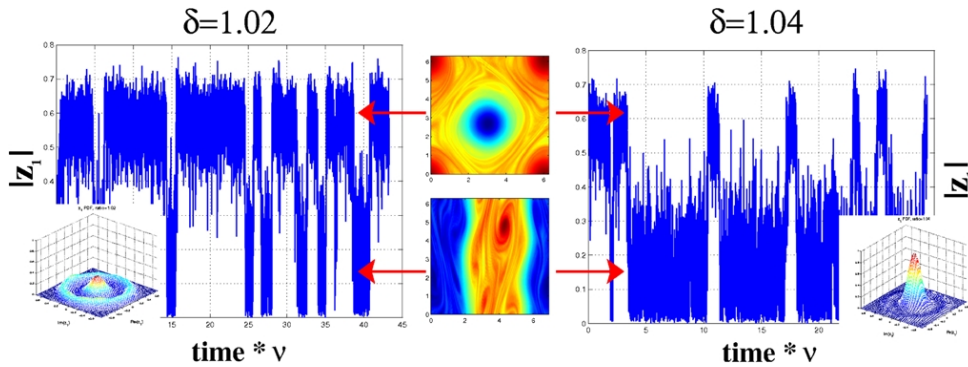


Figure 2. Figure taken from Bouchet & Simonnet (2009) showing time series and probability density functions for the order parameter $z_1 = \omega_{\mathbf{k}}(k_x = 0, k_y = 1)$ illustrating random changes between dipoles and unidirectional flows. The coloured insets show the vorticity fields.

We consider the 2D Navier-Stokes equations with stochastic forcing and linear friction on a doubly periodic domain $\mathcal{D} = [0, 2\pi\delta] \times [0, 2\pi/\delta]$, where δ is the aspect ratio, given by

$$\frac{\partial \omega_{\mathbf{k}}}{\partial t} + (\mathbf{v} \cdot \nabla \omega)_{\mathbf{k}} = -\mu \omega_{\mathbf{k}} - \nu \lambda_{\mathbf{k}} \omega_{\mathbf{k}} + \sqrt{2\sigma} f_{\mathbf{k}} \eta_{\mathbf{k}} \quad (2a)$$

$$\nabla \cdot \mathbf{v}(\mathbf{x}) = 0 \quad (2b)$$

where the velocity \mathbf{v} is related to the vorticity ω and stream function ψ by

$$\mathbf{v} = \mathbf{e}_z \times \nabla \psi, \quad \omega = \Delta \psi, \quad \omega(\mathbf{x}) = \sum_{\mathbf{k}} \omega_{\mathbf{k}} e_{\mathbf{k}}. \quad (2c)$$

Here $\omega_{\mathbf{k}}$ are the Fourier coefficients of the vorticity on the basis $e_{\mathbf{k}}$ of the Laplacian operator such that $-\lambda_{\mathbf{k}} e_{\mathbf{k}} = \Delta e_{\mathbf{k}}$. $\eta_{\mathbf{k}}$ are considered to be independent Gaussian white noises for each wave number \mathbf{k} : $\langle \eta_{\mathbf{k}}(t) \rangle = 0$, $\langle \eta_{\mathbf{k}}(t) \eta_{\mathbf{k}'}(t') \rangle = \delta_{\mathbf{k}\mathbf{k}'} \delta(t - t')$ with forcing profile $f_{\mathbf{k}}$ normalized by $\sum_{\mathbf{k}} |f_{\mathbf{k}}|^2 / |\mathbf{k}|^2 = 1$.

The corresponding action $S(\omega)$ for Eq. (2) is given by

$$S(\omega) = \frac{1}{2} \int_0^T dt L(\omega, \dot{\omega}) = \frac{1}{2} \int_0^T dt 4\pi^2 \sum_{\mathbf{k}=0}^{\infty} \left[\frac{|\dot{\omega}_{\mathbf{k}} + (\mathbf{v} \cdot \nabla \omega)_{\mathbf{k}} + \mu \omega_{\mathbf{k}} + \nu \lambda_{\mathbf{k}} \omega_{\mathbf{k}}|^2}{|f_{\mathbf{k}}|^2} \right], \quad (3)$$

where $L(\omega, \dot{\omega})$ is the corresponding Lagrangian for the dynamics.

Accordingly, the dynamics of the instanton trajectory can be derived from the corresponding Euler-Lagrange equations of the Lagrangian in Eq. (3). Moreover, as the Lagrangian is explicitly independent of time, Noether's theorem implies that the instanton trajectory will conserve an instanton energy $\mathcal{H}_{\text{Instanton}}$ given by

$$H_{\text{instanton}} = \sum_{\mathbf{k}} \dot{\omega}_{\mathbf{k}} \frac{\partial L}{\partial \dot{\omega}_{\mathbf{k}}} - L. \quad (4)$$

4. The numerical method

One approach to calculating the instanton trajectory would be to apply a shooting method to solve the boundary value problem associated to the Euler-Lagrange dynamics. However, we will approach from a variational point of view, whereby we will systematically minimize the action simultaneously over space and time whilst fixing the two boundary states $\omega_{\mathbf{k}}(t=0)$ and $\omega_{\mathbf{k}}(t=T)$ during the minimization. To handle the action numerically, we must discretize time with N_t grid points, such that $t_j = j\Delta t$ with $0 \leq j < N_t$ and $\Delta t = T/N_t$ and consider a finite number N of Fourier modes. We implement the mid-point rule for the time derivative, giving the discretized action as

$$S^D(\omega) = 2\pi^2 \Delta t \sum_{j=0}^{N_t} \sum_{\mathbf{k}=0}^N \left[\frac{\left| \frac{\omega_{\mathbf{k},j+1} - \omega_{\mathbf{k},j}}{\Delta t} + (\mathbf{v} \cdot \nabla \omega)_{\mathbf{k},j+\frac{1}{2}} + \mu \omega_{\mathbf{k},j+\frac{1}{2}} + \nu \lambda_{\mathbf{k}} \omega_{\mathbf{k},j+\frac{1}{2}} \right|^2}{|f_{\mathbf{k}}|^2} \right],$$

where $\omega_{\mathbf{k},j} = \omega_{\mathbf{k}}(t_j)$ and $\omega_{\mathbf{k},j+\frac{1}{2}} = (\omega_{\mathbf{k},j} + \omega_{\mathbf{k},j+1})/2$.

Usually, minimization of an action can be efficiently achieved by using Newton or quasi-Newton methods that use the exact value or an approximation of the Hessian of the action. However, in our case, due to the large number of degrees of freedom that we use, these methods involve astronomically large matrices for their implementation. Instead, we use the steepest descent method, a strategy that only requires the knowledge of the first derivative of S . The procedure is defined by a series of guesses to the instanton trajectory $\omega_{\mathbf{k},j}^n$, that are iteratively improved until we are within some tolerance of the true instanton trajectory. At each iteration, the current guess $\omega_{\mathbf{k},j}^n$ is improved by reduction in the direction of the anti-gradient of S , i.e.

$$\omega_{\mathbf{k},j}^{n+1} = \omega_{\mathbf{k},j}^n - \alpha^n \frac{\partial S}{\partial \omega_{\mathbf{k},j}^n},$$

where α^n is a search length that is determined at each iteration such that the new estimate of the instanton trajectory is a better minimizer of S than the previous one. This procedure is iterated over n until $||\partial S / \partial \omega_{\mathbf{k},j}^n|| < \epsilon$, where ϵ is a given tolerance on the derivative.

5. The over-damped limit

To verify that our numerical algorithm works, we consider the over-damped limit, where $\mu, \nu \gg E^{1/2}$, and $E = -\frac{1}{2} \int d\mathbf{x} \omega \psi$ is the energy of ω at a given time. In this limit, the nonlinear

advection term in the 2D Navier-Stokes equation is small compared to the linear friction and viscosity terms. Hence, we may neglect $\mathbf{v} \cdot \nabla \omega$ in the action (3). We stress that this regime is not the regime for observing bistability behaviour, but is used to verify the numerical code. In this case, at leading order, the dynamics is just a Gaussian process and one can explicitly solve the Euler-Lagrange equations for the instanton trajectory giving the instanton solution of

$$\omega_{\mathbf{k}}(t) = \left(\frac{\omega_{\mathbf{k}}(0)e^{-\gamma_{\mathbf{k}}T} - \omega_{\mathbf{k}}(T)}{e^{-\gamma_{\mathbf{k}}T} - e^{\gamma_{\mathbf{k}}T}} \right) e^{\gamma_{\mathbf{k}}t} + \left(\frac{\omega_{\mathbf{k}}(T) - \omega_{\mathbf{k}}(0)e^{\gamma_{\mathbf{k}}T}}{e^{-\gamma_{\mathbf{k}}T} - e^{\gamma_{\mathbf{k}}T}} \right) e^{-\gamma_{\mathbf{k}}t} \quad (5)$$

where $\gamma_{\mathbf{k}} = \mu + \nu \lambda_{\mathbf{k}}$.

We then use the solution (5) to verify the numerical code. We use 32^2 Fourier modes in space and 100 grid points in time with $T = 10$ in a square periodic box ($\delta = 1$). For this example, we set a uniform forcing profile $f_{\mathbf{k}}$ in Fourier space, and set the two end states of our instanton trajectory to be the parallel and dipole states shown in Figs. 3 and 4 respectively.

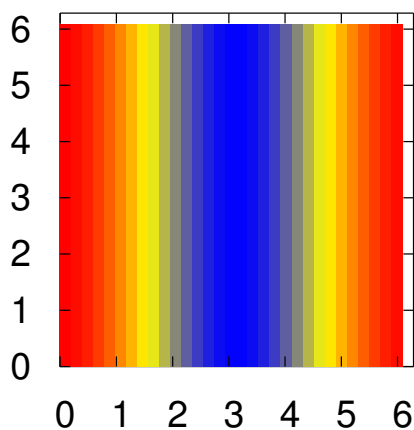


Figure 3. Vorticity profile of the initial state of the instanton trajectory given by $\omega(\mathbf{x}, t = 0) = \frac{1}{\pi} \cos(x)$. Red is positive vorticity and blue is negative vorticity.

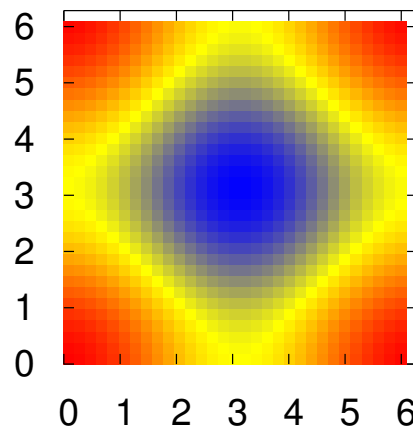


Figure 4. Vorticity profile of the final state of the instanton trajectory given by $\omega(\mathbf{x}, t = T) = \frac{1}{\sqrt{2\pi}} [\cos(x) + \cos(y)]$. Red is positive vorticity and blue is negative vorticity.

These states correspond to the large-scale macrostates of the two metastable states seen in the bistability behaviour of the DNS of the 2D Navier-Stokes equation of Bouchet & Simonnet (2009). Both boundary states are normalized so that both are of unit energy. This gives a characteristic turnover time $\tau \sim 1$. In Fig. 5 we plot the $\text{Re} [\omega_{\mathbf{k}}(k_x = 1, k_y = 0)]$ for the instanton trajectories for two simulations, one with $\mu = 1, \nu = 0$ and another with $\mu = 0.1, \nu = 0$. The numerical results for the instanton trajectory are plotted by points, whilst the corresponding theoretical instanton trajectories, given by Eq. (5), are plotted by solid lines. We observe good numerical agreement to the theoretical results confirming that our numerical code is minimizing to the instanton trajectory. In Fig. 6 we plot the instanton energy defined by Eq. (4) for both simulations. We observe good instanton energy conservation for both simulations..

Furthermore, in the over-damped limit, we can explicitly compute the action:

$$S = 4\pi^2 \sum_{\mathbf{k}} \left| \frac{\omega_{\mathbf{k}}(0)e^{-\gamma_{\mathbf{k}}T} - \omega_{\mathbf{k}}(T)}{e^{-\gamma_{\mathbf{k}}T} - e^{\gamma_{\mathbf{k}}T}} \right|^2 \gamma_{\mathbf{k}} (e^{2\gamma_{\mathbf{k}}T} - 1) \xrightarrow{T \rightarrow \infty} 4\pi^2 \sum_{\mathbf{k}} \gamma_{\mathbf{k}} |\omega_{\mathbf{k}}(T)|^2,$$

which in the limit $T \rightarrow \infty$ only depends on the final state and not the initial state. This is understandable, as over an infinite time it should not ‘cost’ anything for the trajectory to relax

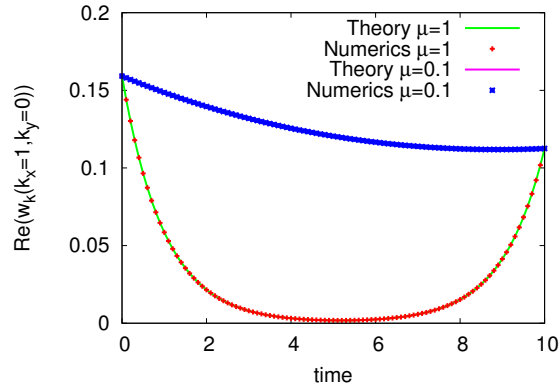


Figure 5. Plot of the evolution of the Fourier mode $\text{Re}(\omega_{\mathbf{k}}(k_x = 1, k_y = 0))$ along the instanton trajectory in the over-damped case with $\mu = 1$ and $\mu = 0.1$. The numerical results (depicted by points) are compared to the theoretical trajectory of Eq. (5) (depicted by solid lines).

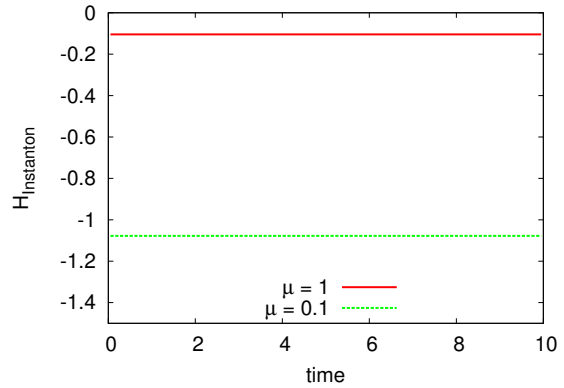


Figure 6. Plot of the instanton energy $\mathcal{H}_{\text{Instanton}}$ for the two simulations with $\mu = 1$ and $\mu = 0.1$. We observe instanton energy conservation in both, indicating that the numerical simulations has approximated the true instanton trajectories well.

to the ground state, with only the trajectory from the ground state to the final state giving a contribution to the action S .

6. The inviscid limit

In the inviscid limit, the 2D Navier-Stokes equations become the 2D Euler equations. In this case, both the initial parallel and final dipole states shown in Figs. 3 and 4 are steady states of the Euler dynamics, i.e. they solve

$$\mathbf{v} \cdot \nabla \omega = 0.$$

Moreover, in the inviscid limit, any two steady states can be connected via a continuous path through an infinite number of steady states. This can be achieved by a trajectory going linearly to zero and vice versa. In such cases, as the instanton time $T \rightarrow \infty$, the action will tend to zero because the trajectory simply diffuses across an energy barrier connected via an infinite number of steady states. This implies that the presence of dissipation is important if we want to observe an instanton trajectory with a non-zero action.

Furthermore, for the Euler dynamics, the action of the instanton trajectory can be expressed as the total time of the instanton trajectory T multiplied by the instanton energy $H_{\text{Instanton}}$ plus boundary terms, more explicitly:

$$S(\omega^*) = TH_{\text{Instanton}} + \sum_{\mathbf{k}} (\dot{\omega}_{\mathbf{k}}^* - (\mathbf{v}^* \cdot \nabla \omega^*)_{\mathbf{k}}) \omega_{\mathbf{k}}^* \Big|_{t=0}^{t=T}$$

This is the consequence of the nonlinear advection term of the 2D Euler equations being homogeneous of order two.

7. The inertial limit with non-zero dissipation

The inertial limit is when we consider the 2D Navier-Stokes equations in the regime of small non-vanishing dissipation and small amplitude forcing, i.e. $\mu, \nu \ll \sigma \ll E^{1/2}$. This corresponds

to the bistability regime. We compute the instanton trajectories between the parallel and dipole states of Figs. 3 and 4. Due to the closeness of the dynamics to inviscid limit, we characterize the distance of the instanton trajectories from the trajectories that go through a continuous set of steady states by observing $\|\mathbf{v} \cdot \nabla \omega\|$ with time. Moreover, we investigate the behaviour of the instanton trajectories as we vary the aspect ratio of the box.

8. Conclusions

In conclusion, we have applied instanton theory to the field of fluid dynamics. We have considered the simplest turbulence model showing bistability and calculated the instanton trajectory between two metastable states. We have presented a numerical scheme to calculate such trajectories for this model and have shown good agreement of the numerical results to the theoretical predictions made in certain regimes.

We have shown that in the limit of zero dissipation and with $T \rightarrow \infty$ limit, the action S will go to zero, and the instanton trajectory will go through a infinite set of continuous steady states of the 2D Euler equations.

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