Rare Event Algorithm Links Transitions in Turbulent Flows with Activated Nucleations

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Many turbulent flows undergo drastic and abrupt configuration changes with huge impacts. As a paradigmatic example we study the multistability of jet dynamics in a barotropic beta plane model of atmosphere dynamics. It is considered as the Ising model for Jupiter troposphere dynamics. Using the adaptive multilevel splitting, a rare event algorithm, we are able to get a very large statistics of transition paths, the extremely rare transitions from one state of the system to another. This new approach opens the way for addressing a set of questions that are out of reach through direct numerical simulations. We demonstrate for the first time the concentration of transition paths close to instantons, in a numerical simulation of genuine turbulent flows. We show that the transition is a noise-activated nucleation of vorticity bands. We address for the first time the existence of Arrhenius laws in turbulent flows. The methodology we developed shall prove useful to study many other transitions related to drastic changes for the turbulent dynamics of climate, geophysical, astrophysical, and engineering applications. This opens a new range of studies impossible so far, and bring turbulent phenomena in the realm of nonequilibrium statistical mechanics.

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Many turbulent flows undergo drastic and abrupt configuration changes with huge impacts [1–7]. Earth's magnetic field reverses on geological timescales due to the turbulent motion of Earth's metal core [3], wall flows transition from laminar to turbulent [7–9], experiments in convection turbulence show bistability [4–6], global climate changes like the glacial-interglacial transitions or the Dansgaard-Oeschger events are related to the turbulent oceans and atmosphere coupled to ice and carbon dioxide dynamics [10]. Is the kinetics and phenomenology of these turbulent transitions analogous to phase transitions in condensed matter and rare conformational changes of molecules in chemistry and biochemistry? These key questions have not been addressed so far because of the difficulty related to the numerical complexity: We need both a proper turbulence representation and to run extremely long simulations to observe transitions. In this Letter we show that a new numerical approach based on rare event algorithms improves exponentially our capabilities. With this tool, we make the first numerical study of metastability and spontaneous transitions for a genuine turbulent dynamics. We study atmospheric turbulent jet transitions, relevant to describe abrupt climate changes on Jupiter's troposphere.

Pictures of Jupiter show fascinating zonal bands whose colors are correlated with the troposphere flow vorticity. Those bands correspond to East-West (zonal) velocity jets, which are stationary for centuries. During the period 1939–1940 a fantastic phenomenon occurred: the planet lost one of its jets [11], which was replaced by three white anticyclones. Phil Marcus subsequently called this event a Jovian sudden climate change [12]. This rare event is one example among thousands of sudden transitions between attractors in the self-organization of billions of vortices in turbulent flows. In this Letter, we study the barotropic beta-plane quasigeostrophic equations: the simplest model that describes the turbulent atmosphere jet self-organization [13–18]. It is the Ising model of atmosphere dynamics: the simplest model to describe jet formation, although too simple to be quantitatively realistic.

The dimensionless versions of the model equations read

$$\partial_t \omega + \mathbf{v} \cdot \nabla \omega + \beta v_y = -\alpha \omega - \nu_n (-\Delta)^n \omega + \sqrt{2\alpha} \eta, \qquad (1)$$

where $\mathbf{v} = \mathbf{e}_z \times \nabla \psi$ is the nondivergent velocity, v_y the North-South velocity component, $\omega = \Delta \psi$ and ψ the vorticity and the stream function, respectively, and α is a linear friction coefficient; see Supplemental Material [19] for the dimensional equations. The noise η forces the flow dynamics and is precisely defined in the Supplemental Material [19]. When $\beta = 0$, those equations are the two-dimensional stochastic Navier-Stokes equations for which a few rare transitions have been observed in the past between the dipole and jet states [20], and for which impressive explicit relation between the energy injection rate and the Reynolds stresses have been recently derived [21–23]. Such relations have been further justified and extended to the

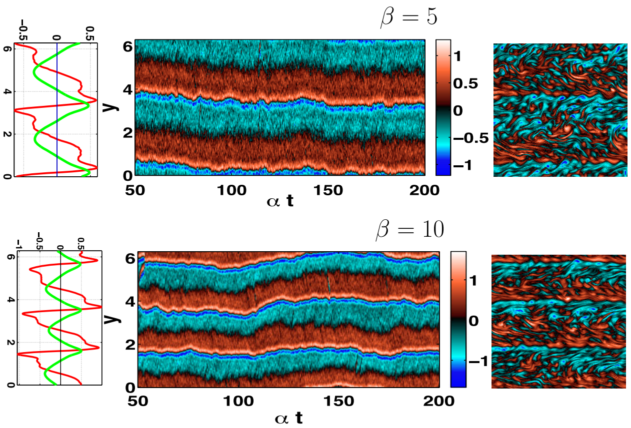

FIG. 1. Right panels: typical snapshots of the vorticity fields (the colors show the vorticity values, with red for positive ones, blue for negative ones and black for intermediate ones; the range of vorticity is $[-1, 1]$). Middle panels: Hovmöller diagrams of zonally averaged vorticity (the horizontal axis is αt, the vertical one is y, and the color represents the x-averaged vorticity, $\alpha = 1.20 \times 10^{-3}$). Left panels: time and zonally averaged vorticity (red) and velocity (green). The top plots show a two jet state for $\beta = 5$, while the bottom ones show a three jet one for $\beta = 10$.

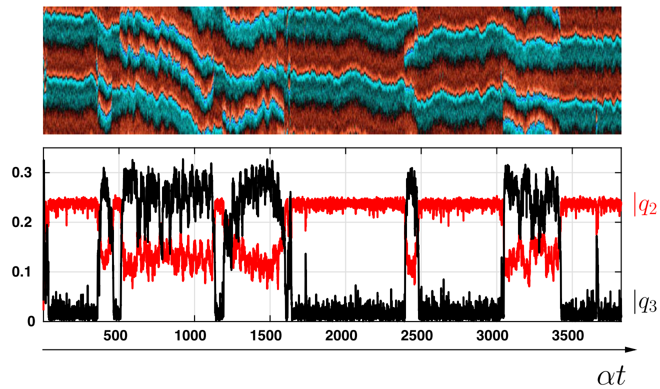

FIG. 2. Rare transitions between turbulent attractors with, respectively, 2 and 3 alternating jets. Upper panel: Hovmöller diagram of the zonal mean vorticity. Lower panel: time series of the modulus of q_2 (red) and q_3 (black), the zonal mean vorticity Fourier components, for wave number 2 and 3, respectively, versus the rescaled time αt ($\alpha = 1.2 \times 10^{-3}$ and $\beta = 5.26$).

case $\beta \neq 0$ [24], see also Ref. [18]. For $\beta \neq 0$ and for small enough α the vorticity dynamics self-organizes into zonal bands like on Jupiter (Fig. 1). The dimensionless parameter β is proportional to β_d that measures the local variations of the Coriolis parameter, and is related to the Rhines scale, defined in the Supplemental Material [19], PDF file. The number of jets roughly scales like $\beta^{1/2}$ [14]. Figure 1 shows metastable turbulent states with either two or three alternating jets, for two different values of β.

When β is increased, one expects to see transitions from attractors with 2 to 3 alternating jets ($2 \to 3$ transitions). As there is no related symmetry breaking, one may expect these transitions to be first order ones with discontinuous jumps of some order parameters. In situations with discontinuous transitions when an external parameter β is changed, one expects for each bifurcation a multistability range (β_1, β_2) in which two (or more) possible states exist for a single value of β. Such a bistability has indeed been observed [16] by changing the model initial conditions. Figure 2 shows for the first time spontaneous transitions between the two bistable states. The transitions are well characterized by the Fourier components $q_n = \int dxdy\omega(x,y)e^{iny}/(2\pi)^2$ for $n = 2$ and $n = 3$: Fig. 2 features five $2 \to 3$ transitions, and five $3 \to 2$ transitions in about 10^6 turnover times.

We would like to address the following basic questions: What are the transition rates? What are the relative probability of each of the attractors (equilibrium constants)? Do the transition trajectories concentrate close to instantons like in statistical physics [25]? Do the thousands of small scale vortices act collectively as atoms in a nucleation process? Unfortunately, such questions are unaffordable using direct numerical simulations. Observing such rare spontaneous transitions in turbulent flows is highly unusual as most turbulent simulations last a few turnover times at most, because of the huge numerical cost. This limitation is a wall that drastically limits the study of transitions in turbulent flows to extremely simple models and a few transitions only. In order to study rare transitions in turbulent flows, we consider a completely new approach in turbulence studies: using the adaptive multilevel splitting algorithm [26–28] (see Fig. 3). This rare event algorithm belongs to the family of splitting algorithms, where an ensemble of trajectories are simulated and subjected to a succession of selections, cloning or killing, and dynamical mutation steps. The principle of the algorithm [26] is described in the legend of Fig. 3. A full description of the algorithm and of the method to compute transition rates is described in Ref. [28]. Its mathematical properties (convergence, fluctuations, etc) have been studied recently [27,29]. This algorithm was first tested in extremely simple dynamics with few degrees of freedom [26]. It has been applied for the first time to a partial differential equation, the Ginzburg-Landau dynamics, in Ref. [28]. In Ref. [28], for the equilibrium Ginzburg-Landau dynamics, a very precise comparison of the AMS algorithm results with explicit analytic results of the Freidlin-Wentzell theory is performed, showing that the algorithm can faithfully compute averaged transition times of order of 10^{15} larger than the typical duration of a direct numerical simulation. This Letter describes the first application of the adaptive multilevel splitting algorithm to turbulent flows, and to complex nonequilibrium dynamics, where analytical results are out of reach. This is also the first use of a rare event algorithm to study transitions in turbulence that cannot be studied through direct numerical simulations. Using this algorithm we have been able to compute thousands of spontaneous transitions and their probability. Table I shows

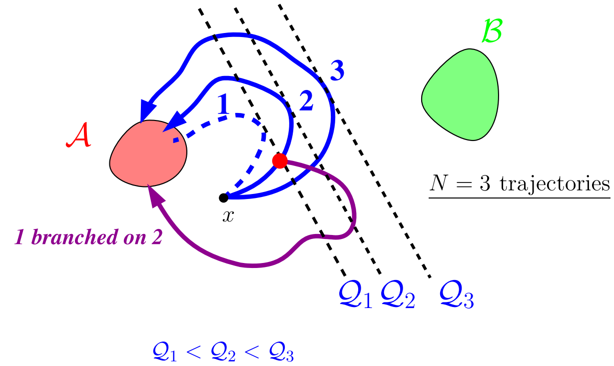

FIG. 3. (a) Sketch of the adaptive multilevel splitting (AMS) algorithm, one of the most versatile rare event algorithms. The aim of the algorithm is to compute the very small probability to go from a set $\mathcal{A}$ (for instance a two jet state) to a set $\mathcal{B}$ (for instance a three jet state). N initial trajectories are computed from the model (N is typically a few thousands). A score function $\mathcal{Q}$ measures how far each trajectory goes in the direction of $\mathcal{B}$. The worst trajectory is deleted (trajectory No. 1 on the sketch). It is replaced by a new trajectory (purple trajectory) whose initial condition is picked from one of the other previous trajectories (trajectory 2 on the sketch) at the time (red dot on the sketch) when it was crossing the $\mathcal{Q}$ level with the maximum value of $\mathcal{Q}$ for the deleted trajectory. This last step is called resampling or cloning. As the new set of N trajectories has been obtained by selecting $N-1$ trajectories among N, and computing a new trajectory which has the same probability as the $N-1$ other ones, the new set has a probability $1-1/N$. The resampling step is iterated K times, leading to a new trajectory set with probability $(1-1/N)^K$. This very efficiently produces extremely rare transitions from one attractor to another and gives an unbiased estimate of their probability (see the Supplemental Material [19], PDF file for more precise explanations).

the exponential reduction of computational time in order to compute thousands of transitions.

Figure 4 and the associated movie (Supplemental Material [19], video) describe $2 \to 3$ transitions for $\alpha = 6.0 \times 10^{-4}$. Both the movie and the figure clearly illustrate that a new jet formation proceeds through the nucleation of two new ensembles of small positive and negative vortices lying in an area of overall zero vorticity located at a westward jet. Like in condensed matter, such a nucleation is highly improbable. Indeed a too small new vortex band is unstable. However, when exceptionally, by chance, a critical size is reached, the new band becomes stable and will last for an extremely long time. In combination with this growth, the three jets move apart. It is striking to note that all nucleations ($2 \to 3$ transitions) have been observed at the edge of westward jets, and all coalescences ($3 \to 2$ transitions) occurred at the edge of eastward jets. This phenomenology is illustrated on an even clearer way on Fig. 5(a) that shows a typical zonal velocity evolution during the nucleation of new jet and Fig. 5(b) that shows jet coalescence.

TABLE I. CPU time [days (d), years (yr)] needed to obtain 1000 transition paths using 200 processors for the adaptive multilevel splitting algorithm compared to direct numerical simulation for different values of α.

α	AMS	DNS
1.2×10^{-3}	1.0 d	15 d
0.9×10^{-3}	1.4 d	210 d
0.6×10^{-3}	2.2 d	~51 yr
0.45×10^{-3}	3.4 d	~2050 yr

The Arrhenius law, from thermodynamics and statistical physics, states that transitions rates are proportional to $\lambda \propto \exp(-\Delta V/\alpha)$, where ΔV is either a free energy, an entropy, or a potential difference, and α is related to thermal or non-thermal noises. This classical law describes transitions in many fields of physics, chemistry, biology, statistical, and quantum mechanics. Could it be relevant to turbulence problems, extremely far from equilibrium? This fascinating hypothesis has never been tested for turbulent flows because this requires a huge number of rare transitions for different values of α, an impossible task without a rare event algorithm. The validity of this hypothesis is suggested by the nucleation phenomenology. Moreover, we have recently conjectured [30,31] that the slow evolution of the zonally averaged part of the flow, $U(y,t) = \int dx \mathbf{v}(x,y,t)$, may be described by an effective equation

$$\frac{\partial U}{\partial \tau} = F(U) + \sqrt{\alpha}\sigma(U,\tau), \tag{2}$$

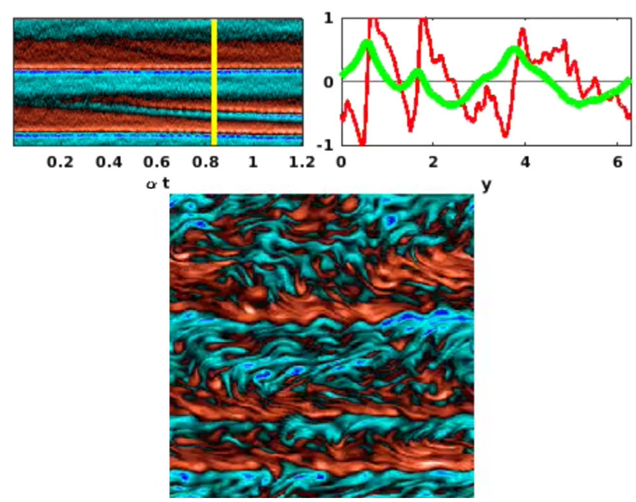

FIG. 4. Nucleation of a new jet. The panels display the same quantities as Fig. 1. A set of vortices is able to nucleate a new band of blue vorticity, a very unlikely process, leading to the birth of a new jet seen on the green velocity curve. As in nucleation processes in condensed matter, once the nucleated structure is large enough the new jet will be stable and persist for extremely long times, as seen on the Hovmöller diagram (see also the Supplemental Material [19], video).

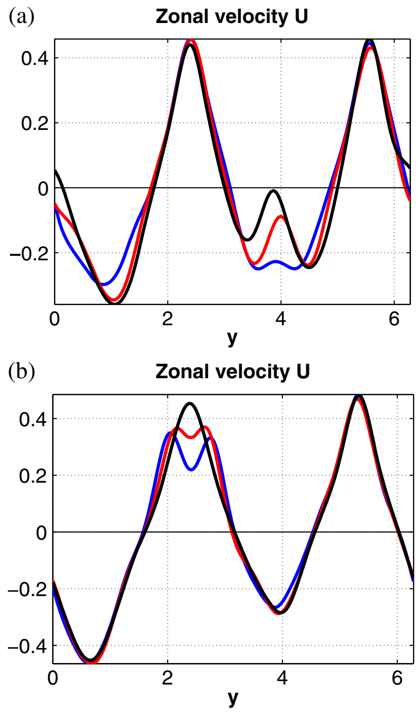

FIG. 5. (a) Zonally averaged velocity during the nucleation of a third jet in a $2 \to 3$ jet transition: The blue, red and black curves show the velocity field at the start, at an intermediate stage, and at a more advanced stage of the nucleation, respectively. (b) Zonally averaged velocity during the coalescence of two jets in a $3 \to 2$ transition: The blue, red and black curves show the velocity field before, just before, and after the merging, respectively. These 4 plots illustrate that while transitions appear at random time, their dynamic is predictable.

where $\tau = \alpha t$ is a rescaled time, $F(U)$, the average of the divergence of the Reynolds stress [more precisely, Ref. [30] derived Eq. (2) formally and proved that the hypothesis for the asymptotic expansion leading to $F(U)$ are self-consistent, while Ref. [31] explained how to compute $\sigma(U, \tau)$]. The classical Freidlin-Wentzell theory [32] describes large deviations and rare transitions for Eq. (2) for weak noises ($\alpha \ll 1$). From this theory, two main consequences can be derived from Eq. (2): first an Arrhenius law, and second a concentration of transition paths close to a single path called instanton [25,33,34] (see Ref. [3] for an experimental observation in a magnetohydrodynamics turbulent flow, and Ref. [34] for numerical results for Burger's equation). In the remainder of the Letter we will show that these two consequences are verified, giving further support to Eq. (2).

Using the adaptive multilevel splitting algorithm, we have been able to collect thousands of transition paths. In Fig. 6, 80% of the direct $2 \to 3$ transitions are inside the red tube, and 80% of the direct$3 \to 2$ trajectories are inside the blue tube, in the reduced space of observables ($|q_2|$, $|q_3|, |q_4|$) (see Fig. 2). This unambiguously illustrates the concentration of transition paths close to an instanton. This is the first demonstration of such a phenomenology from

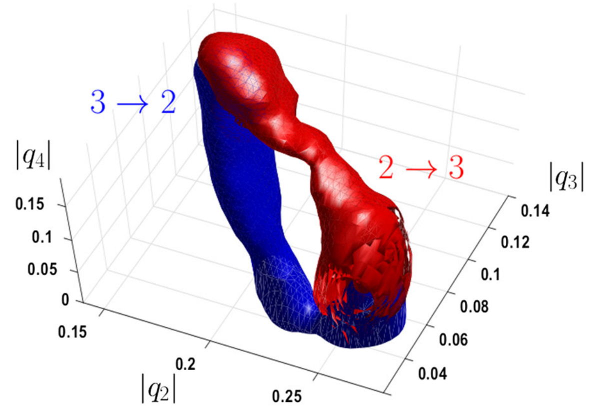

FIG. 6. Instantons: The reactive tubes corresponding to the distribution of transition paths for the $2 \to 3$ (red) and $3 \to 2$ (blue) transitions. They illustrate the concentration of transition paths typical of an instanton phenomenology (see the main text) ($\beta = 5.26$ and $\alpha = 1.2 \times 10^{-3}$).

numerical simulations in a turbulent flow. We stress the strong asymmetry between the $2 \to 3$ and $3 \to 2$ transition, which is expected for an irreversible dynamics of a turbulent flow. We also study for the first time in a turbulent flow an Arrhenius law, based on thousands of extremely rare transitions (see Table I). Following the approach described in Ref. [35] we compute the averaged transition time $\mathbb{E}(T) = 1/\lambda$ for the $2 \to 3$ transitions (see Fig. 7). Those data are clearly compatible with an Arrhenius law $\log \mathbb{E}(T) \propto \Delta V/\alpha$. Viscosity effects are discussed in the Supplemental Material [19], PDF file.

The new use of the adaptive multilevel splitting algorithm for studying rare transitions in a turbulent flow demonstrates for the first time that thousands of vortices can self-organize and nucleate new structures and trigger transitions. Like in condensed matter, the transition paths concentrate close to instantons. Instantons may be used as

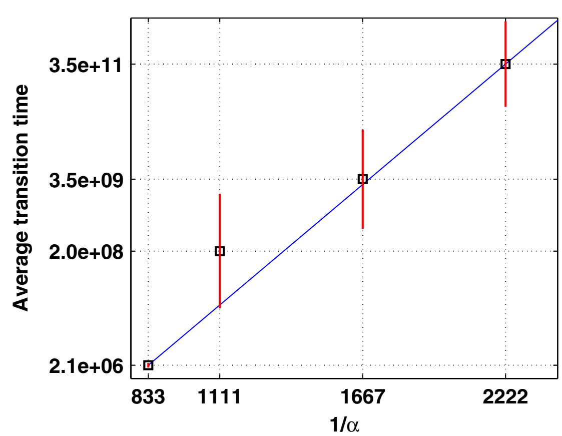

FIG. 7. Arrhenius law. Logarithm of the mean first transition time T from the two-jet to the three-jet attractors versus $1/\alpha$ ($\beta = 5.5$). This result suggests that mean transition times might follow an Arrhenius law $T \propto e^{\Delta U/\alpha}$.

precursors stressing that the extremely rare transition became more probable. A very important future work will be the study of Jupiter' s abrupt climate changes with models that are more realistic then the barotropic β-plane model [36]. While it is unlikely that the same nucleation phenomenology should hold for all possible turbulent transitions, the methodology developed will prove useful to study many other transitions related to drastic changes for climate, geophysical, astrophysical, and engineering applications. This opens a new range of studies impossible so far, and brings turbulent phenomena in the realm of nonequilibrium statistical mechanics. Examples include the Kuroshio current bistability, weather regime changes in meteorology, regime transitions in the Sun superficial dynamics, astrophysical magnetic field transitions, and bistability in turbulent boundary layer detachments.

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