Rare events and large deviation theory for turbulent flows

F. BOUCHET – ENS de Lyon and CNRS
With E. SIMONNET and J. ROLLAND (Jupiter's climate change) and E. LEVEQUE and T. LESTANG (extreme drags).

NCTR – Les Houches – February 2021.

Outline

1. Rare events in complex dynamics and turbulent flows
   - Rare events with a huge impact: extreme heat waves and extreme drags
   - Abrupt climate changes and transitions between turbulent attractors
   - Instanton theory and predictability of dynamical paths that lead to rare events
2. Jupiter's abrupt climate changes and instantons
   - Multistability for the dynamics of Jupiter jets
   - The Adaptive Multilevel Splitting (AMS) rare event algorithm
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   - Drag statistics for 2D turbulent flow
   - Predictability of flow patterns for extreme drags
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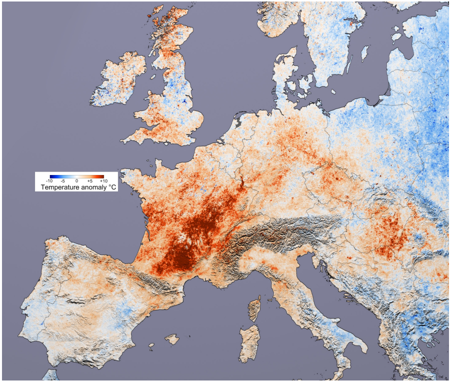
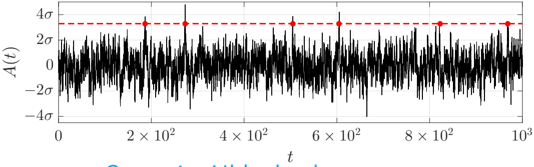
Extreme Heat Waves

Example: the 2003 heat wave over western Europe

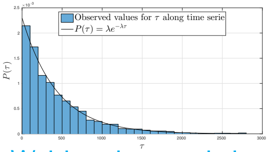


July 20 2003-August 20 2003 land surface temperature minus the average for the same period for years 2001, 2002 and 2004 (TERRA MODIS).

Extreme Events, Poisson Statistics, and Return Times



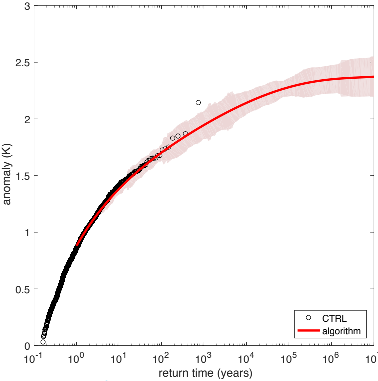
Ornstein–Uhlenbeck extremes



Waiting time statistics

For systems with a single state, rare enough events are uncorrelated and have a Poisson statistics

The Return Times of Extreme Heat Waves



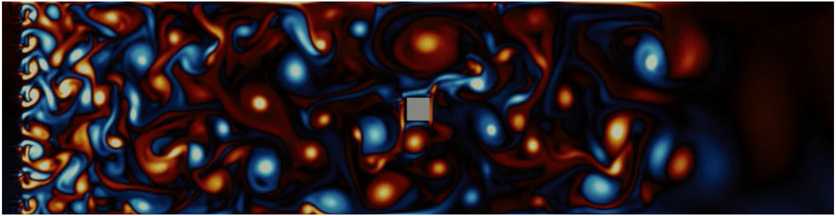
Return time of 90 day European heat waves

F. Ragone, J. Wouters, and F. Bouchet, PNAS, 2018

Extreme Forces on Objects Embedded in Turbulent Flows

Thibault Lestang's PhD thesis.

Lattice Boltzmann Simulations of 2D Flows



Vorticity ($Re_G = 1\,200$, $Re_O \simeq 500$) (T. Lestang's PhD work)

Click on the image for runing the movie

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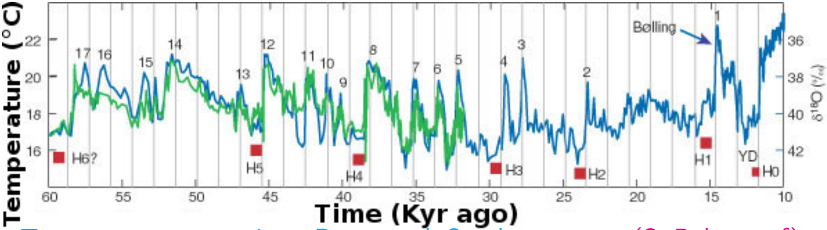
Abrupt Climate Changes (Last Glacial Period)

Long times matter

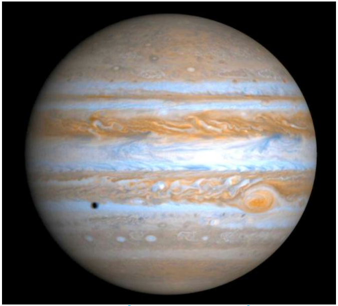


Temperature versus time: Dansgaard–Oeschger events (S. Rahmstorf)

- What is the dynamics and probability of abrupt climate changes?

Jupiter's Zonal Jets

An example of a geophysical turbulent flow (Coriolis force, huge Reynolds number, ...)



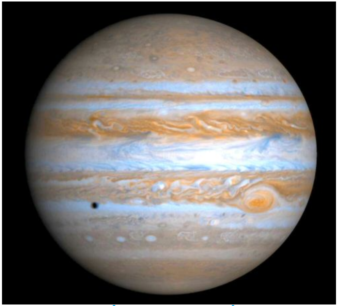
Jupiter's troposphere

Jupiter's animation (Voyager)

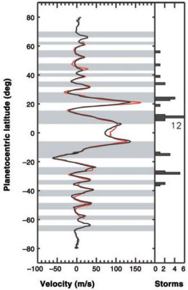
Click on the image for runing the movie

Jupiter's Zonal Jets

We look for a theoretical description of zonal jets



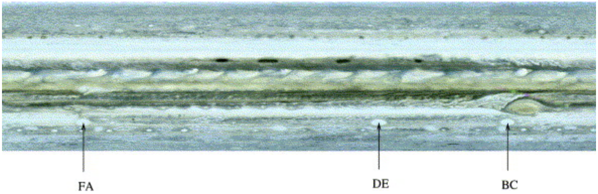
Jupiter's troposphere

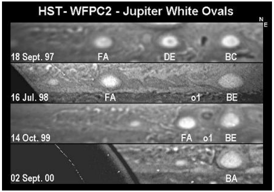


Jupiter's zonal winds (Voyager and Cassini, from Porco et al 2003)

Jupiter's Abrupt Climate Change

Have we lost one of Jupiter's jets ?





Jupiter's white ovals (see Youssef and Marcus 2005)

The white ovals appeared in 1939-1940 (Rogers 1995). Following an instability of one of the zonal jets?

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Freidlin–Wentzell Theory

$$\frac{dx}{dt} = \mathrm{b}(x) + \sqrt{2\varepsilon}\eta(t)$$

- Path integral representation of transition probabilities:

$$P(x_t, T; x_0, 0) = \int_{x(0)=x_0}^{x(T)=x_T} \mathrm{e}^{-\frac{\mathscr{A}_T[x]}{\varepsilon}} \mathscr{D}[x]$$

$$\text{with } \mathscr{A}_T[x] = \int_0^T \mathscr{L}[x,\dot{x}]\, dt \text{ and } \mathscr{L}[x,\dot{x}] = \frac{1}{4}[\dot{x} - \mathrm{b}(x)]^2.$$

- We may consider the $\varepsilon \to 0$ limit, using a saddle point approximation (WKB), Then we obtain the large deviation result

$$P(x_T, T; x_0, 0) \underset{\varepsilon \to 0}{\asymp} e^{-\frac{\min_{\{x(t)\}}\left\{\mathscr{A}_T[x]\middle| x(0)=x_0 \text{ and } x(T)=x_T\right\}}{\varepsilon}}.$$

Most Transition Paths Follow the Instanton

- In the weak noise limit, most transition paths follow the most probable path (instanton)

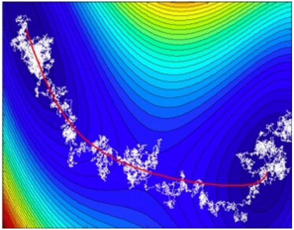


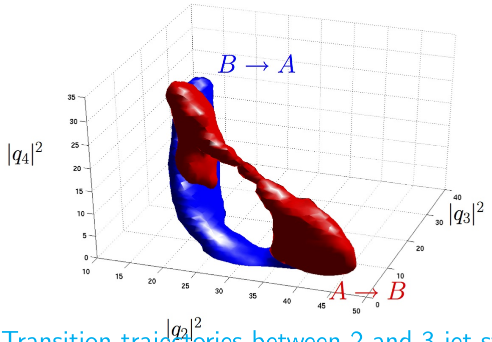
Figure by Eric Van den Eijnden

- For gradient dynamics, instantons are time reversed relaxation paths from a saddle to an attractor. Arrhenius law then follows

$$P(x_1, T; x_{-1}, 0) \underset{k_B T_e \to 0}{\asymp} \mathrm{e}^{-\frac{\Delta V}{k_B T_e}}.$$

Atmosphere Jet "Instantons" Computed using the AMS

AMS: an algorithm to compute rare events, for instance rare reactive trajectories

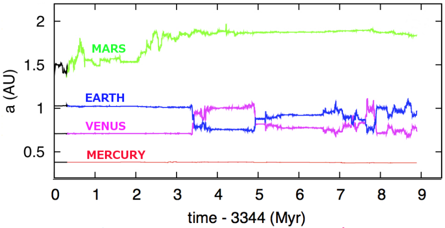


Transition trajectories between 2 and 3 jet states

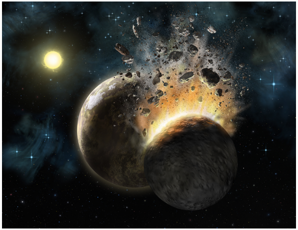
- The dynamics of turbulent transitions is predictable.
- Asymmetry between forward and backward transitions.

F. Bouchet, E. Simonnet and J. Rolland, Phys. Rev. Lett., 2019.

Instantons and Collisional Trajectories in the Solar System



Distance from the sun vs time (J. Laskar)
(7.10^6 hours of CPU, p=1/100 000)



Collision probability?

- Do the collisional trajectories of the solar system follow an instanton?

E. Woillez and F. Bouchet, Phys. Rev. Lett., 2020 and Nature Review Physics 2020.

Rare Events in Complex Dynamics

The scientific questions:

- What is the probability and the dynamics of those rare events?
- Is the dynamics leading to such rare events predictable?
- How to sample rare events, their probability, and their dynamics?
- Are direct numerical simulations a reasonable approach?
- Can we devise new theoretical and numerical tools to tackle these issues?

Large Deviation Theory

- Large deviation theory is a general framework to describe probability distribution in asymptotic limits

$$P\left[X_{\varepsilon}=x\right] \underset{\varepsilon \ll 1}{\asymp} \mathrm{e}^{-\frac{\mathscr{F}[x]}{\varepsilon}}.$$

For equilibrium statistical mechanics, $\mathscr{F}$ is the free energy, and $\varepsilon = k_B T/N$.

Maths: Cramer 30', Sanov 50', Lanford 70', Freidlin–Wentzell 70' and 80', Varadhan, ... In parallel with theoretical physicist ideas.

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The Barotropic Quasi-Geostrophic Equations

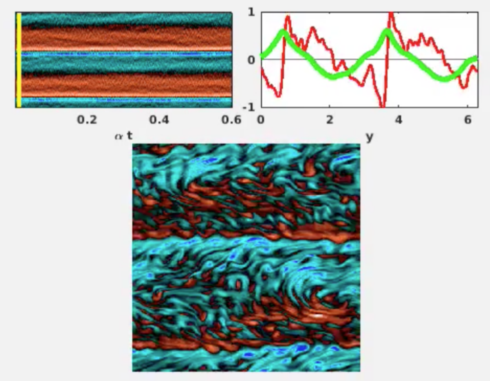
- The simplest model for geostrophic turbulence.
- Quasi-Geostrophic equations with random forces

$$\frac{\partial q}{\partial t} + \mathbf{v}.\nabla q = \nu \Delta \omega - \alpha \omega + \sqrt{2\alpha} f_s,$$

where $\omega = (\nabla \wedge \mathbf{v}).\mathbf{e}_z$ is the vorticity, $q = \omega + \beta y$ is the Potential Vorticity (PV), β is the Coriolis parameter, f_s is a random Gaussian field with correlation $\langle f_S(\mathbf{x},t) f_S(\mathbf{x}',t') \rangle = C(\mathbf{x}-\mathbf{x}')\delta(t-t')$.

- A reasonable model for Jupiter's zonal jets.

Dynamics of the Barotropic Quasi-Geostrophic Equations



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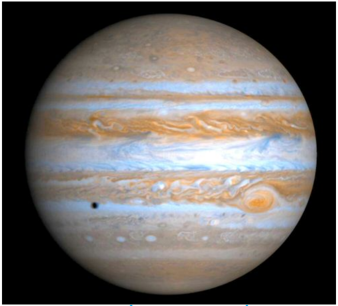
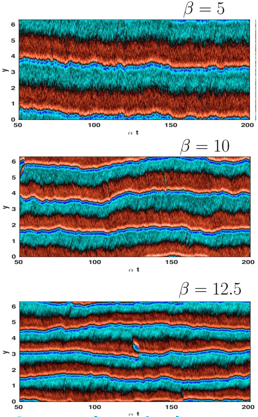
Top: Zonally averaged vorticity (Hovmöller diagram and red curve) and velocity (green). Bottom: vorticity field

Multistability for Quasi-Geostrophic Jets



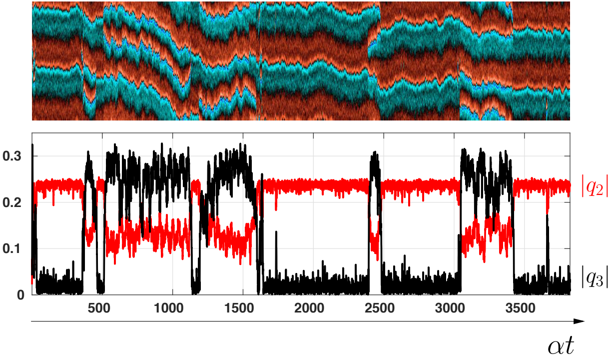
Jupiter's atmosphere



QG zonal turbulent jets

- Multiple attractors had been observed previously by B. Farrell and P. Ioannou.

Rare Transitions Between Quasigeostrophic Jets



Rare transitions for quasigeostrophic jets (with E. Simonnet)

- This is the first observation of spontaneous transitions.
- How to predict those rare transitions? What is their probability? Which theoretical approach?

Kinetic Theory of the Slow Evolution of Zonal Jets

- We have derived a slow jet equation and justified averaging (ergodicity, etc ...), (Bouchet, Nardini and Tangarife, 2013, J. Stat. Phys.).
- The rare transitions involve non-Gaussian fluctuations of the Reynolds stress. (Bouchet, Grafke. Tangarife and Vanden-Eijnden, 2016, J. Stat. Phys.).
- We have computed the large deviations of Reynolds stress that explain rare transitions (Bouchet, Marston and Tangarife, 2018, Phys. Fluids).

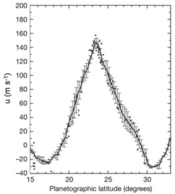
http://perso.ens-lyon.fr/freddy.bouchet/

An Explicit and Local Formula for the Reynolds Stress

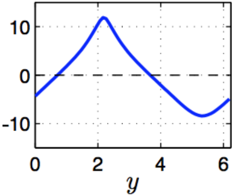
$$\frac{\partial U}{\partial \tau} = F(U)$$

- For small scale forces we have an explicit expression for $F(U)$

$F(U) = -\frac{\partial}{\partial y}\left(\frac{\varepsilon}{\partial U/\partial y}\right) - \alpha U,$ where ε is the energy injection rate.



Jupiter's velocity profile (Sanchez Lavega, 2008)



Theoretical/numerical velocity profile

E. Woillez and F. Bouchet, EPL 2017 and JFM, 2018

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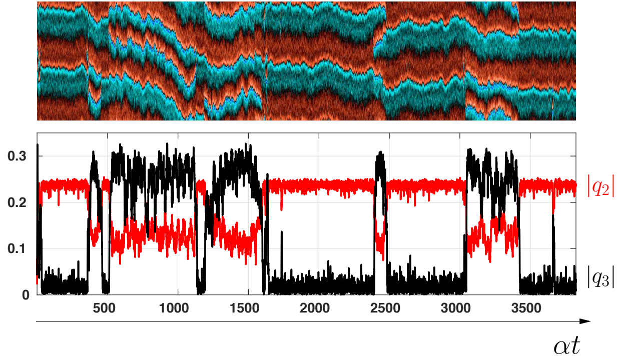

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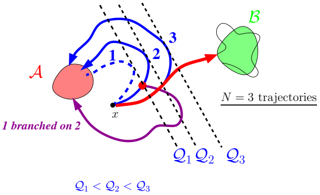
Rare Events and Adaptive Multilevel Splitting (AMS)

AMS: an algorithm to compute rare events, for instance rare transition paths

- Rare event algorithms: Kahn and Harris (1953), Chandler, Vanden-Eijnden, Schuss, Del Moral, Dupuis, ...
- The adaptive multilevel splitting algorithm:



AMS algorithm

Strategy: selection and cloning.
Probability estimate:

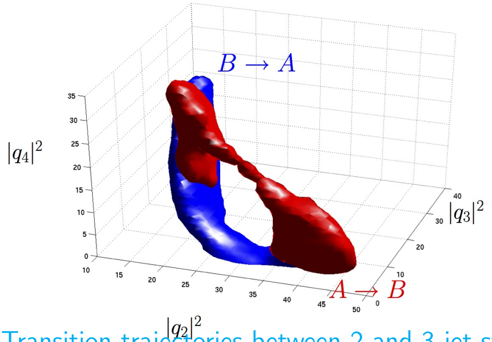
$$\hat{p} = (1 - 1/N)^K, \text{ where}$$

N is the clone number and K the iteration number.

Cérou, Guyader (2007). Cérou, Guyader, Lelièvre, and Pommier (2011).

Atmosphere Jet "Instantons" Computed using the AMS

AMS: an algorithm to compute rare events, for instance rare reactive trajectories

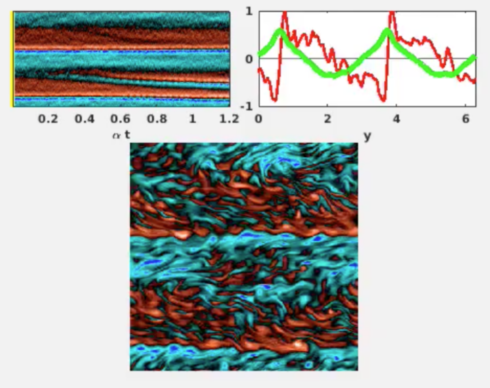


Transition trajectories between 2 and 3 jet states

- The dynamics of turbulent transitions is predictable.
- Asymmetry between forward and backward transitions.

F. Bouchet, J. Rolland and E. Simonnet, 2019, PRL.

A Transition from 2 to 3 Jets



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Top: Zonally averaged vorticity (Hovmöller diagram and red curve) and velocity (green). Bottom: vorticity field

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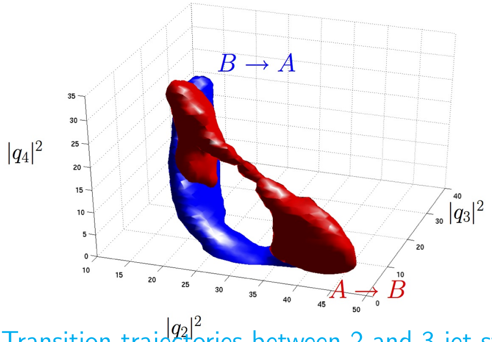

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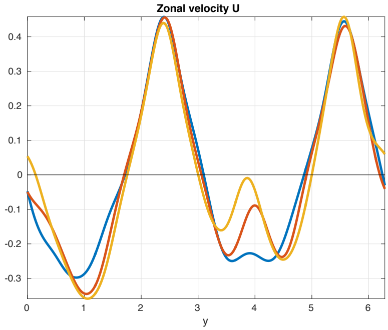
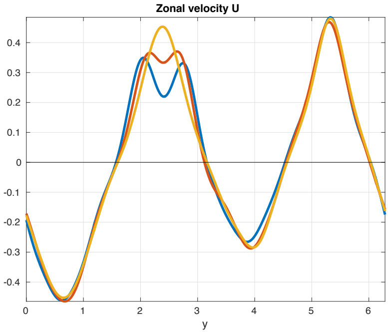
Evolution of Velocity Fields During the Transition





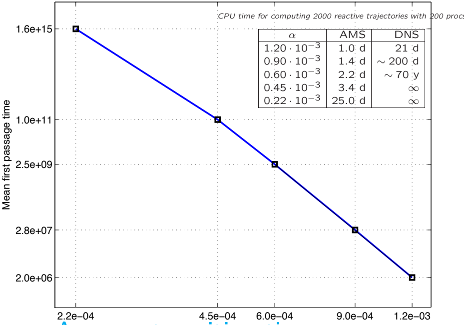
Nucleation of a new jet

Merging of two jets

- Asymmetry between forward and backward transitions.

Transition Rates for Unreachable Regimes Through DNS

With the AMS we can estimate huge average transition times

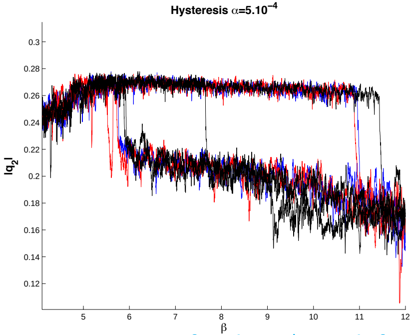


α	AMS	DNS
$1.20 \cdot 10^{-3}$	1.0 d	21 d
$0.90 \cdot 10^{-3}$	1.4 d	$\sim$ 200 d
$0.60 \cdot 10^{-3}$	2.2 d	$\sim$ 70 y
$0.45 \cdot 10^{-3}$	3.4 d	∞
$0.22 \cdot 10^{-3}$	25.0 d	∞

Average transition time versus α

- With the AMS algorithm, we study transitions that would require an astronomical computation time using direct numerical simulations.

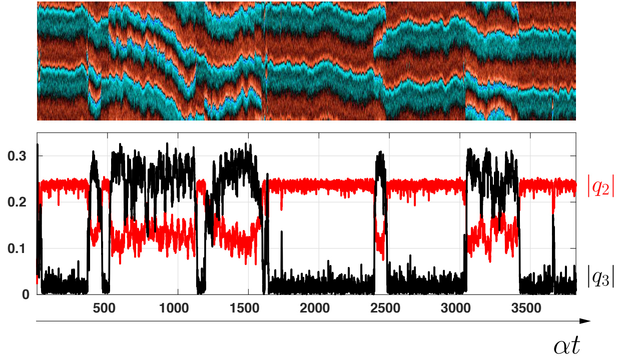
A Complex Internal Dynamics for the 3-Jet States



Hysteresis experiment for the 2/3 jet bifurcations

- The 3 jet states have larger fluctuations than the 2 jet states.

Rare Transitions Between Quasigeostrophic Jets

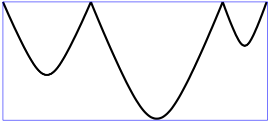


Rare transitions for quasigeostrophic jets

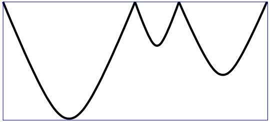
- It seems that the 3 jet states might have different structures.

A Family of Different 3-Jet Attractors

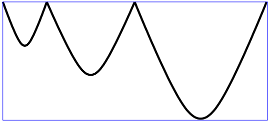
Symmetry breaking within the set of 3-jet attractors



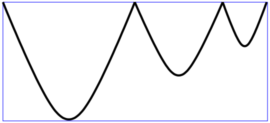
$(\sigma_1, \sigma_2, \sigma_3)$



$(\sigma_2, \sigma_3, \sigma_1)$



$(\sigma_3, \sigma_1, \sigma_2)$



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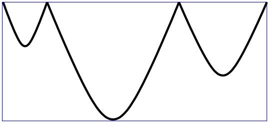

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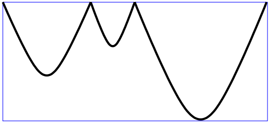
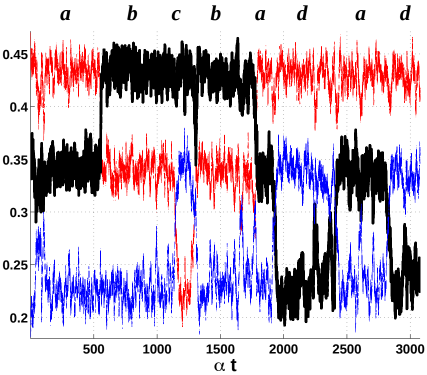


$(\sigma_1, \sigma_3, \sigma_2)$

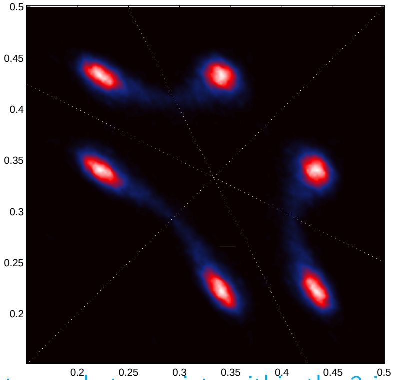
Schematic zonal velocity fields $U(y)$ for the 3-jet attractors

Internal Multistability for the 3-Jet Attractors



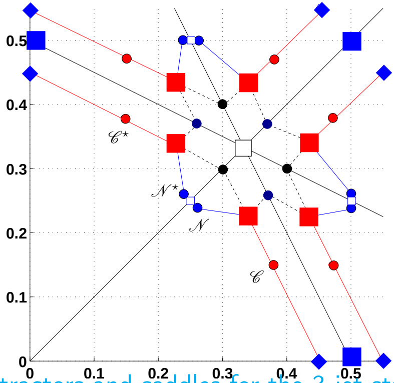
Timeseries for the distance between jets within the 3-jet attractors

Internal Multistability for the 3-Jet Attractors



PDF of distances between jets within the 3-jet attractors.

Bifurcation Diagram for the 3-Jet Attractors



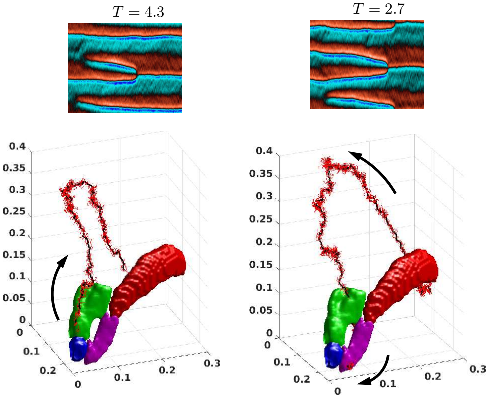
Attractors and saddles for the 3 jet states

Each axe represent one of the 3 distances between the 3 jets.

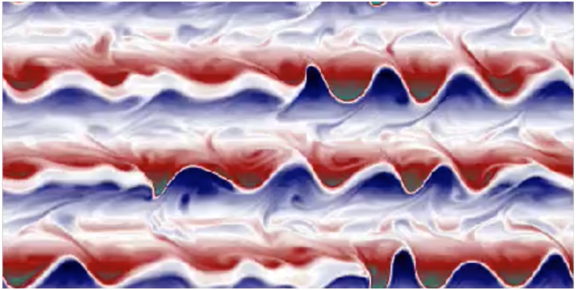
F. Bouchet, J. Rolland and E. Simonnet, submitted to JAS

A Richer Transition Phenomenology

Transitions through states with four jets are possible



A Transition in a 2-Layer QG model



Click on the image for runing the movie

Potential vorticity in a 2-layer QG model ($H_1/H_2 = 1$, $R/L_x = 0.01$, $L_y/L_x = 0.5$)

Conclusions (Jupiter's abrupt climate change)

- We have computed rare transitions between zonal jets, similar to Jupiter's abrupt climate changes, that can not be computed using direct numerical simulations. Transitions follow instantons and Arrhenius laws. (with J.R. and E.S.).
- We have partial results for the justification of averaging (ergodicity, etc ...), (with C.N., and T.T.).
- For small scale forces, the average Reynolds stress can be computed explicitly and is local. We have a good qualitative agreement with Jupiter's jets. (with E.W.).
- The rare transitions involve non-Gaussian fluctuations of the Reynolds stress. (with T.G., T.T., and E. V-E).
- There is a rich phenomenology of internal states for the 3-jet attractors (with E.S. and J.R.).

http://perso.ens-lyon.fr/freddy.bouchet/

Outline

1. Rare events in complex dynamics and turbulent flows
   - Rare events with a huge impact: extreme heat waves and extreme drags
   - Abrupt climate changes and transitions between turbulent attractors
   - Instanton theory and predictability of dynamical paths that lead to rare events
2. Jupiter's abrupt climate changes and instantons
   - Multistability for the dynamics of Jupiter jets
   - The Adaptive Multilevel Splitting (AMS) rare event algorithm
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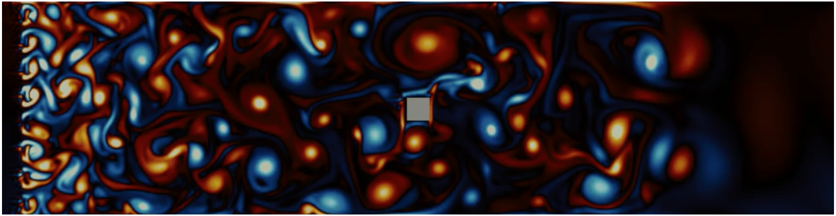
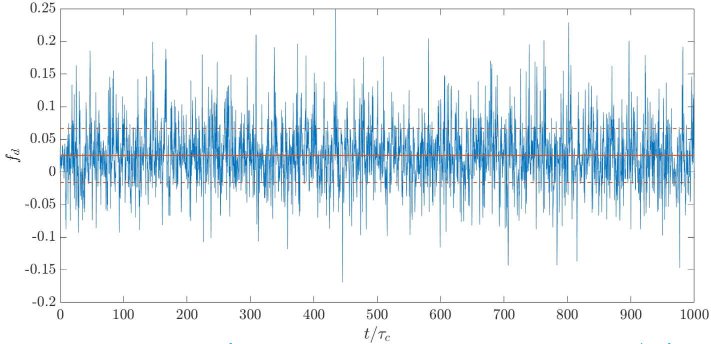
Lattice Boltzmann Simulations of 2D Flows



Click on the image for runing the movie

Vorticity ($Re_G = 1200$, $Re_O \simeq 500$) (T. Lestang's PhD work)

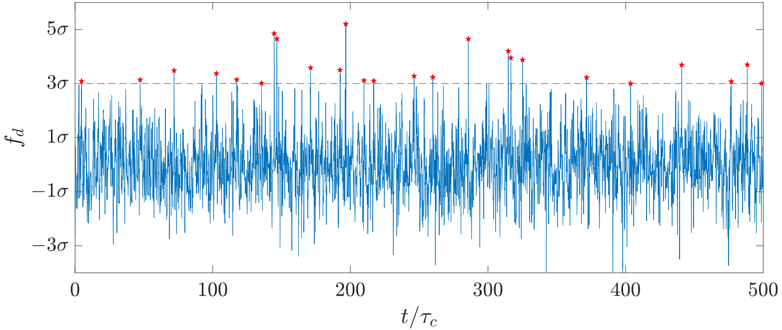
Drag Timeseries for 2D Grid Turbulent Flows



Drag timeseries ($Re_G = 1\,200$, $Re_O \simeq 500$, $\tau_C \simeq L/U$)

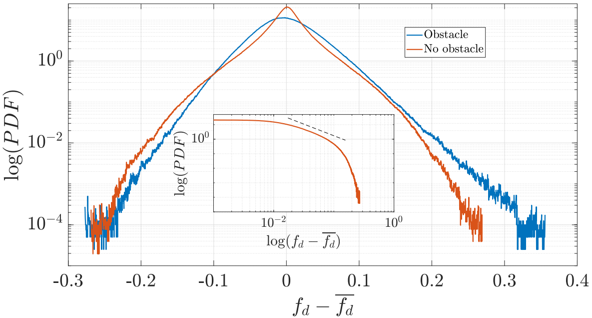
- The drag has quite often negative values ($f_d < \sigma$).

Extreme Drags for 2D Grid Turbulent Flows



Drag extremes

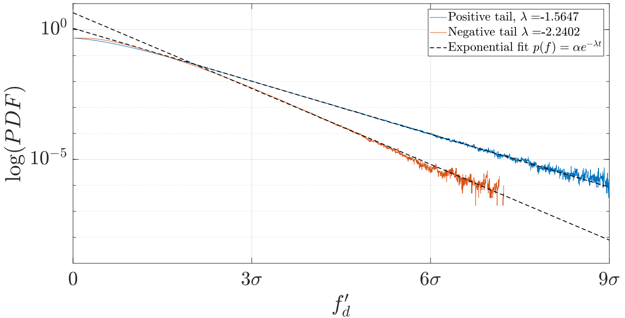
Drag PDF



Drag PDF with and without the obstacle

- The interaction flow/obstacle, besides changing the drag average, increases extreme positive values.

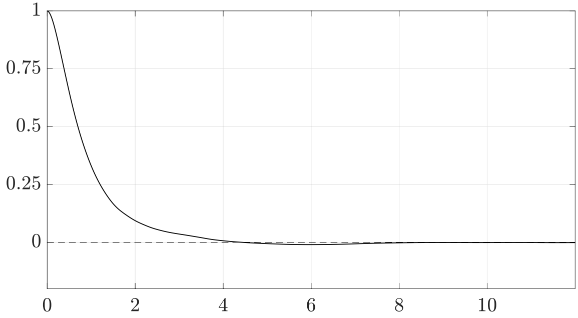
Drag PDF Tail Asymmetry



Drag PDF tails

- Positive drag extremes are more frequent than negative ones.

Drag Autocorrelation Function



Drag autocorrelation Function ($\tau_C \simeq L/U$)

- We observe a fast decrease of correlations.

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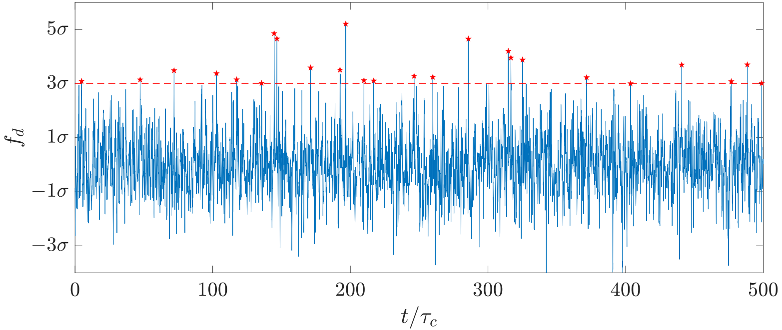
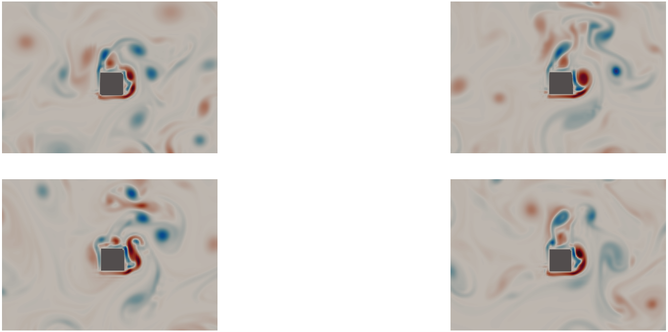
Extreme Drags for 2D Grid Turbulent Flows



Drag extremes

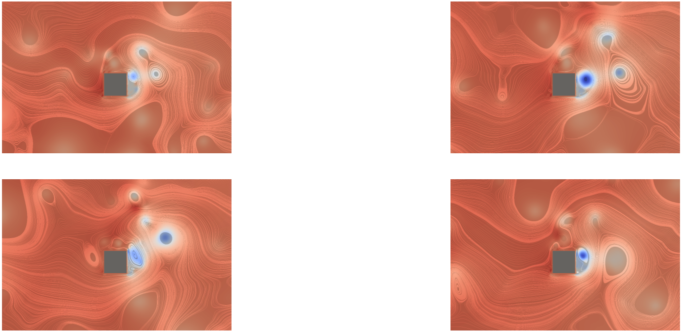
Predictability of Extreme Patterns for Turbulent Flows



Vorticity for the four events with the most extreme drag

- Extreme event patterns are often predictable. Instanton?

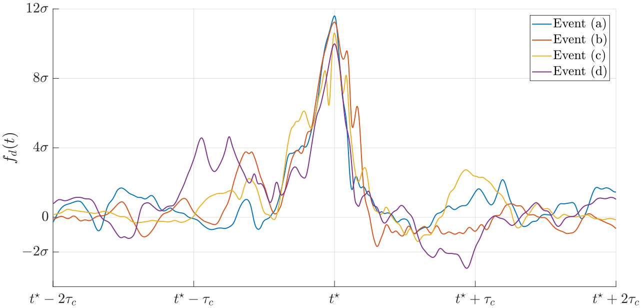
Predictability of Extreme Patterns for Turbulent Flows



Streamlines and pressure for the four events with the most extreme drag

- Extreme event patterns are often predictable. Instanton?

Dynamics for the 4 Most Extreme Drag Events



Drag timeseries for the 4 most extreme

- The extreme dynamics is fast and does not figure persistent features.

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Time Averaged Drag

- For many applications, what matters is the time average:

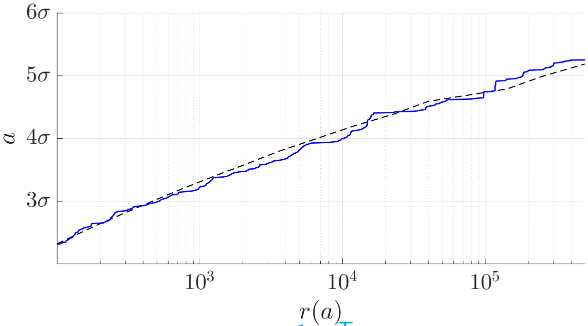
$$F = \frac{1}{T}\int_0^T f_d(t)\,\mathrm{dt}$$

- For example, for a car

$$\tau_c \simeq \frac{L}{U} \simeq \frac{3\,\mathrm{m}}{30\,\mathrm{m.s}^{-1}} = 0.1\,\mathrm{s}.$$

- The meaningful values of T depends on the applications.

Return Times for the Extreme Integrated Drags



Return times for $F = \frac{1}{T}\int_0^T f_d(t)\,\mathrm{d}t$ $(T = 10\tau_c)$

- What is the phenomenology of the extreme integrated drags?

Large deviations for time averaged observables

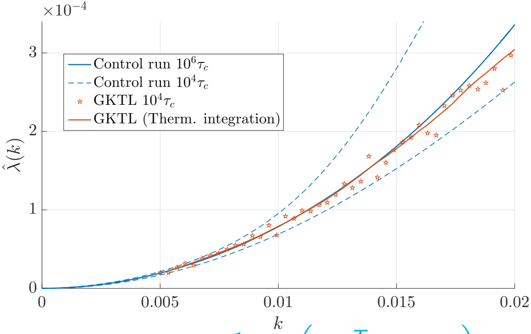
- Donsker–Varadhan: large time asymptotics for time averaged observables.
- Time averaged observables

$$P\left[\frac{1}{T}\int_0^T f_d(t)\,\mathrm{d}t = a\right] \underset{T\to\infty}{\asymp} C\mathrm{e}^{-TI(F)}.$$

- $I(F)$ is the large deviation rate function, related to the scaled cumulant generating function $\lambda(k)$ through

$$I(F) = \sup_k \{Fk - \lambda(k)\}$$

Computing rare time-averaged drags with rare event algorithms

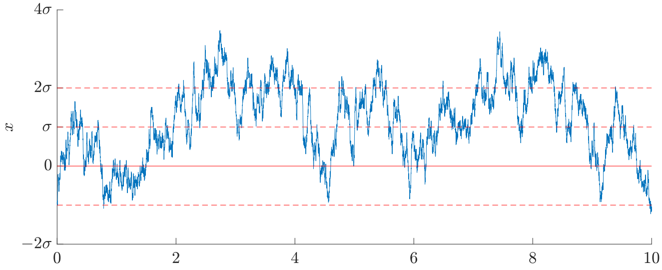


$$\lambda(k) = \lim_{T\to\infty} \frac{1}{T} \exp\left(k \int_0^T f_d(t)\,\mathrm{d}t\right).$$

- The GKTL algorithm is a rather efficient way to compute the large deviation rate function.

Phenomenology of Extremes of Time Averaged Quantities

$\mathrm{d}x = -x dt + \sqrt{2}\mathrm{d}W_t$, (Gaussian stationary PDF - fastdecorrelation).

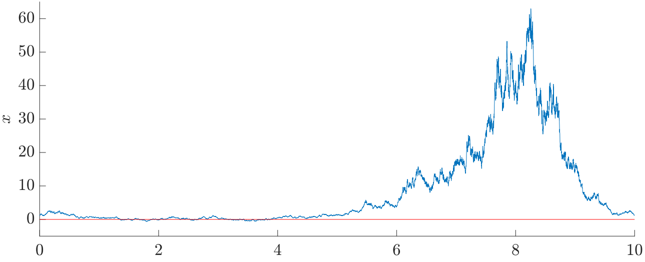


One extreme of $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$, with $T = 10\tau_c$,

- For Gaussian PDF, all times contribute more or less equally to the extreme sum (distributed contribution).

Phenomenology of Extremes of Time Averaged Quantities

$\mathrm{d}x = -x dt + \sqrt{2a(x)}\mathrm{d}W_t$, (PDF with an algebraic tail -fastdecorrelation).



One extreme of $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$, with $T = 10\tau_c$,

- For algebraic tails, a single event dominate the sum (local contribution).

Phenomenology of Extremes of Time Averaged Quantities

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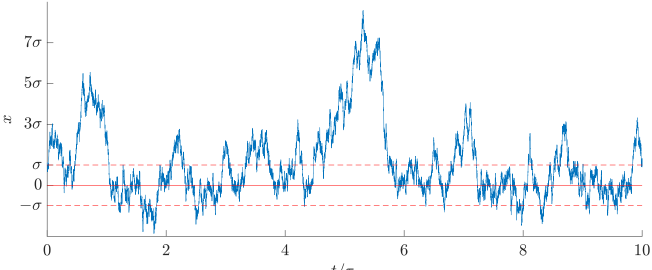


One extreme of $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$, with $T = 10\tau_c$,

- For exponential tails, there is no clear preference for localized or distributed contributions to the extreme sum.

Extremes of a Sum of I.I.D. Random Variables

$$S_N = \frac{1}{N}\sum_{n=1}^{N} X_n$$

- $\{X_n\}_{0\leq n\leq N}$ are N independent and identically distributed random variables with probability distribution function P.
- We consider realizations such that $S_N = a$, where a is a very rare value. Given this condition, what is the typical distribution of $\{X_n\}_{1\leq n\leq N}$. There are two opposite scenario:

1. All X_ns takes values which are close to a, such that $S_N = a$ (scenario probability p_1);
2. One of the X_n takes a very large value Na and the other take typical values close to zero, such that $S_N = a$ (probability p_2).

Extremes of a Sum of I.I.D. Random Variables

1. All X_ns takes values which are close to a, such that $S_N = a$ (scenario probability p_1);
2. One of the X_n takes a very large value Na and the other take typical values close to zero, such that $S_N = a$ (probability p_2).

There are three possible cases:

1. P asymptotically decreases much faster than an exponential (for instance P has Gaussian tails). Then $p_1 \gg p_2$ (all events contribute more or less equally to the sum).
2. P asymptotically decreases much slower than an exponential (for instance P has algebraic tails). Then $p_1 \ll p_2$ (a single event dominate the sum).
3. P tails are asymptotically exponential. This is the marginal case.

Langevin Dynamics and Time Averaged Observables

$$\mathrm{d}x = -xdt + \sqrt{2a(x)}\mathrm{d}W_t$$

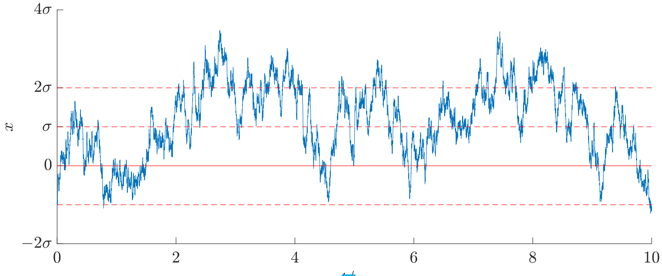
We consider 3 cases:

- $a(x) = 1$; then $P_S(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$.
- $a(x) \underset{x\to\infty}{\sim} \frac{x^2}{\alpha}$; then $P_S(x) \underset{x\to\infty}{\sim} \frac{C}{x^\alpha}$.
- $a(x) \underset{x\to\infty}{\sim} \frac{x}{\alpha}$; then $P_S(x) \underset{x\to\infty}{\sim} \exp(-\alpha x)$.
- For all 3 cases, the decorrelation of x is fast.

What is the phenomenology of the extremes of the time average $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$?

Phenomenology of Extremes of Time Averaged Quantities

$\mathrm{d}x = -x dt + \sqrt{2}\mathrm{d}W_t$, (Gaussian stationary PDF - fastdecorrelation).

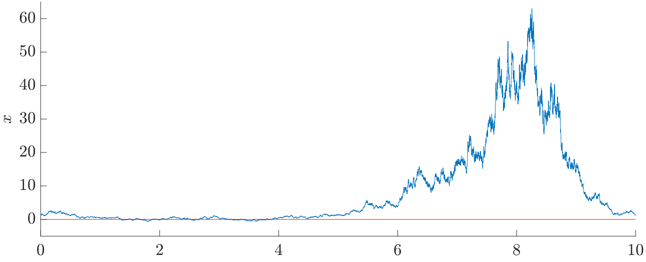


One extreme of $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$, with $T = 10\tau_c$,

- For Gaussian PDF, all times contribute more or less equally to the extreme sum (distributed contribution).

Phenomenology of Extremes of Time Averaged Quantities

$\mathrm{d}x = -x dt + \sqrt{2a(x)}\mathrm{d}W_t$, (PDF with an algebraic tail -fastdecorrelation).



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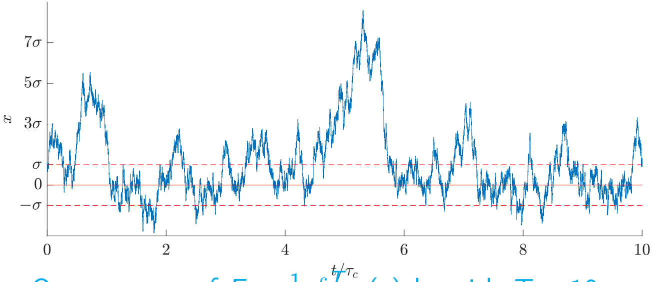

One extreme of $F = \frac{1}{T}\int_0^T x(t)\,\mathrm{d}t$, with $T = 10\tau_c$,

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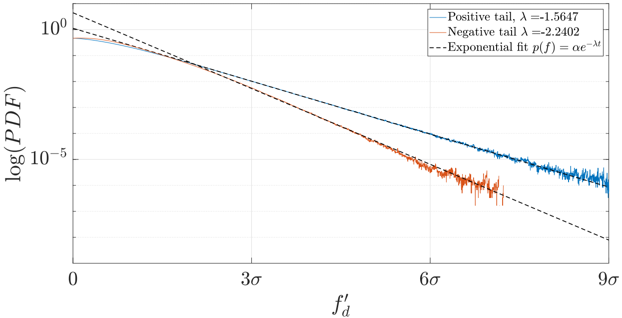
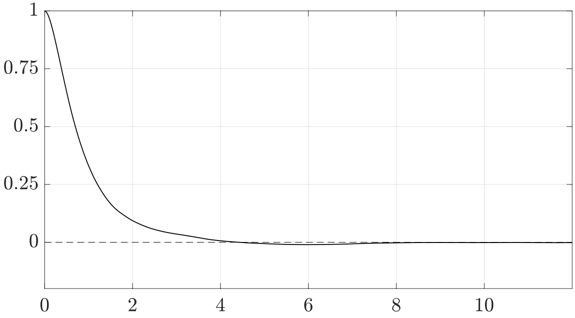
The Drag PDF Tail is Exponential



Drag PDF tails

- The drag PDF tail is close to exponential.

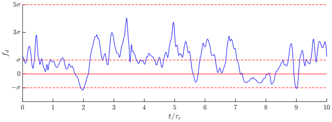
Drag Autocorrelation Function

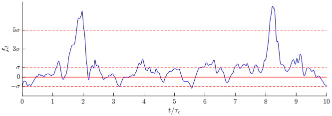


Autocorrelation Function ($\tau_C \simeq L/U$)

- We observe a fast decrease of correlations.

Phenomenology of Extremes of the Time Averaged Drag





Two example for extremes of $F = \frac{1}{T}\int_0^T f_d(t)\,\mathrm{d}t$, with $T = 10\tau_c$ ($F = 4.7\sigma$ and $F = 4.5\sigma$, respectively).

- For extremes of the time averaged drag, there is no clear preference for localized or distributed contributions of the drag.

Extreme Drags: Conclusions

- Drag timeseries are highly fluctuating, with a fast decorrelation and a PDF with exponential tails.
- Very extremes drags seem to be produced by similar events, that involve an extreme low pressure created by a vortex, which is maintained by a transient streamline cap.
- Time averaged drags can be efficiently studied using rare event algorithms, although their performances for this problem is less impressive compared to other applications.
- The phenomenology of long time averaged drag is diverse with a combination of long duration distributed high drag values and localized more intense ones.

T. Lestang, F. Bouchet and E. Lévêque, JFM, 2020

T. Lestang, E. Lévêque et F. Bouchet, to be submitted to JSTAT, 2021