Rare event computations and machine learning for climate dynamics

F. BOUCHET – ENS de Lyon and CNRS
With J. WOUTERS and F. RAGONE (climate heat waves), J. ROLLAND and E. SIMONNET (geostrophic jets)

Journées Calcul et Apprentissage – Lyon – April 2019.

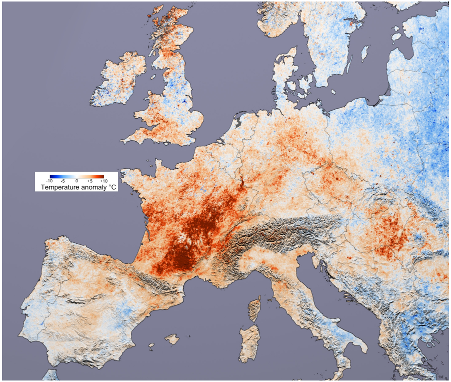
ENS DE LYON
European Research Council
Established by the European Commission

Outline

Outline

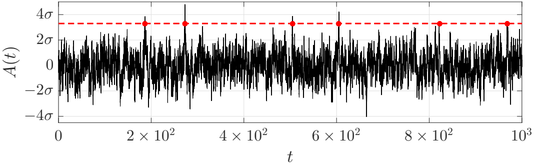
Extreme Heat Waves

Example: the 2003 heat wave over western Europe

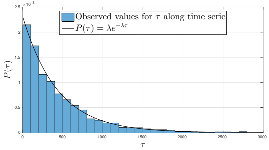


July 20 2003-August 20 2003 land surface temperature minus the average for the same period for years 2001, 2002 and 2004 (TERRA MODIS).

Extreme Events, Poisson Statistics, and Return Times



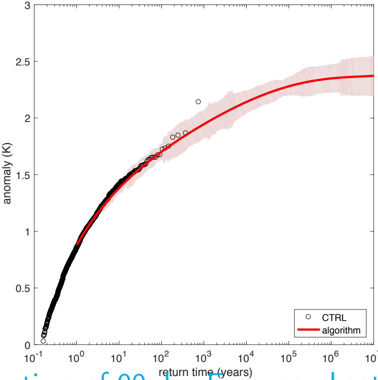
Ornstein–Uhlenbeck extremes



Waiting time statistics

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

The Return Time of Extreme Heat Waves



Return time of 90 day European heat waves

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

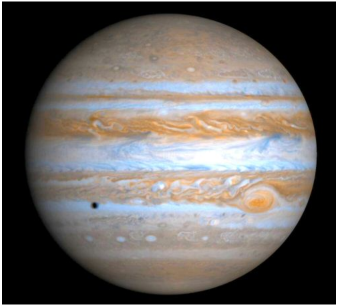
T. Lestang, F. Ragone, C.H. Brehier, C. Herbert, and F. Bouchet, JSTAT, 2018

Outline

1. Rare events in complex dynamical systems
   - Rare events with a huge impact: extreme heat waves
   - Abrupt climate changes and transitions between turbulent attractors
   - Rare and extreme events in astronomy
2. Probability and dynamics of extreme heat waves
   - The jet stream, blocking events, and heat waves
   - Sampling extreme heat waves using a large deviation algorithm
3. Rare transitions for geostrophic jets
   - Freidlin–Wentzell theory
   - Barotropic jet multistability

Jupiter's Zonal Jets

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

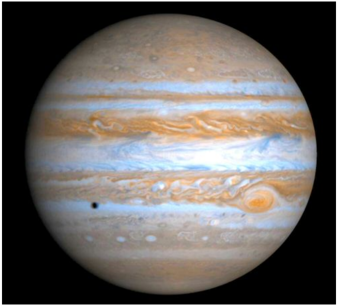


Jupiter's troposphere

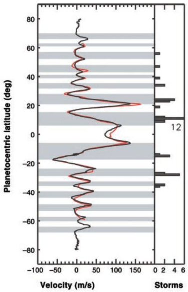
Jupiter's motions (Voyager)

Jupiter's Zonal Jets

We look for a theoretical description of zonal jets



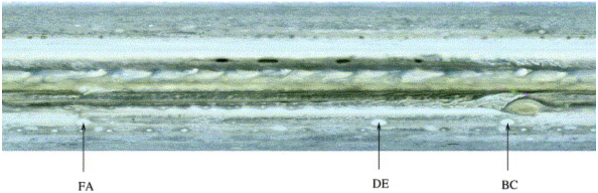
Jupiter's troposphere

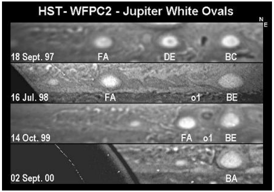


Jupiter's zonal winds (Voyager and Cassini, from Porco et al 2003)

Jupiter's Abrupt Climate Change

Have we lost one of Jupiter's jets ?





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

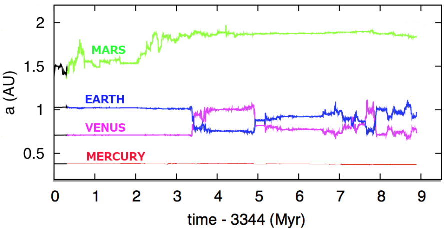
The white ovals appeared in 1939-1940 (Rogers 1995). Following an instability of one of the zonal jets?

Outline

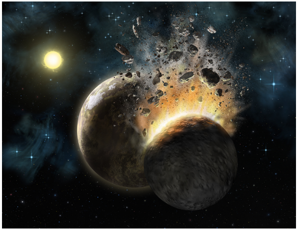
1. Rare events in complex dynamical systems
   - Rare events with a huge impact: extreme heat waves
   - Abrupt climate changes and transitions between turbulent attractors
   - Rare and extreme events in astronomy
2. Probability and dynamics of extreme heat waves
   - The jet stream, blocking events, and heat waves
   - Sampling extreme heat waves using a large deviation algorithm
3. Rare transitions for geostrophic jets
   - Freidlin–Wentzell theory
   - Barotropic jet multistability

Collisional Trajectories in the Solar System

In collaboration with J. Laskar.



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



Collision probability?

- What are the probabilities of past and future qualitative changes of the solar system?

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

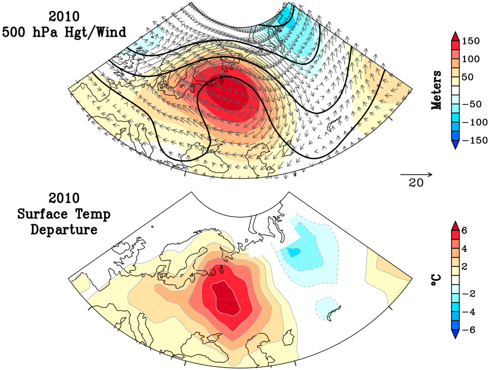
$$P\left[X_{\varepsilon}=x\right] \underset{\varepsilon \ll 1}{\asymp} \mathrm{e}^{-\frac{\mathscr{F}[x]}{\varepsilon}}.$$

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.

Outline

Extreme Heat Waves and Anticyclonic Anomalies

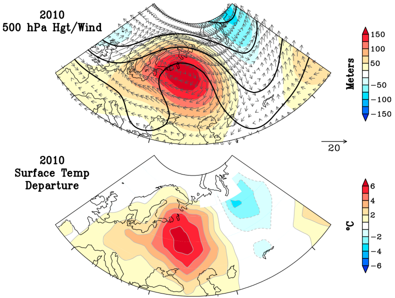


2010 Heat Wave over Eastern Europe (Dole and col., 2011)

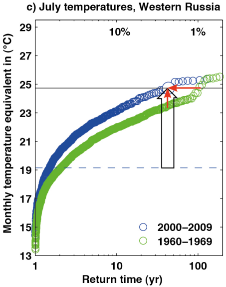
The Jet Stream, Rossby Waves, and Blocking Events

Higher troposphere winds (NASA)

Anthropogenic Causes of the 2010 Heat Wave



(Dole et al., 2011)



Return time of monthly temperature

(Otto et al., 2012)

- A clear anthropogenic impact.
- What are the dynamical mechanisms for such extreme events?

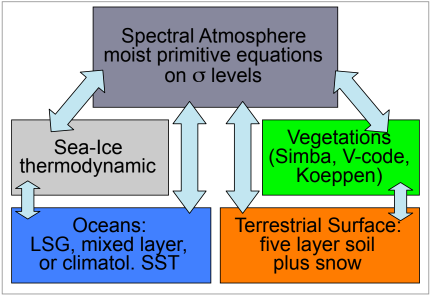
How to Study 10 000 Year Heat Waves with a 200 Year Computation?

Sampling rare events in dynamical systems

The scientific questions:

- What is the probability and the dynamics of those rare events?
- How to sample rare events?
- Are direct numerical simulations a reasonable approach?

Model: the Planetary Simulator (Plasim) - Hamburg



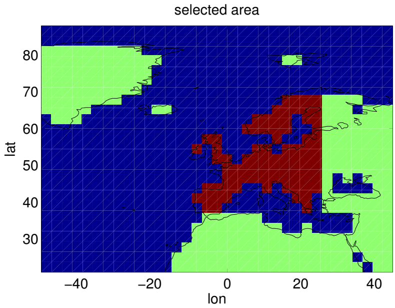
Plasim main properties

- We use the Planet Simulator (PlaSim) model (an Earth system model of intermediate complexity) developed at Hamburg.
- T42 horizontal resolution (64x128 grid points), 10 vertical layers, about $10^5 - 10^6$ degrees of freedom.

Plasim Northern Hemisphere Dynamics

500 HPa geopotential height and temperature anomalies

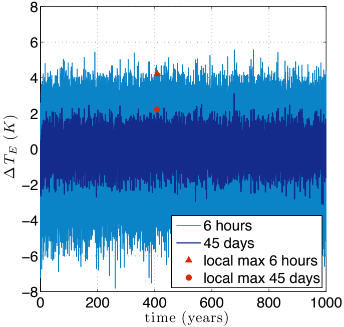
Observable: Averaged Surface Temperature



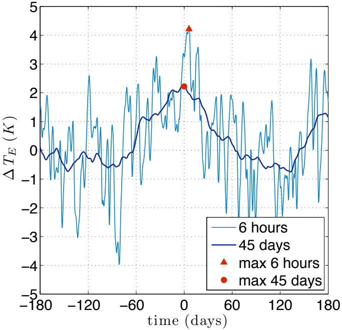
The observable will be Europe averaged surface temperature

$$a = \frac{1}{T}\int_0^T \mathrm{d}t \, \langle Temp \rangle_{\mathrm{Europe}}(t)$$

45-Day Averaged Temperature over Europe (Plasim Model)



Full timeseries



Close to a heat wave

$$a = \frac{1}{T}\int_0^T \mathrm{d}t\, \langle Temp \rangle_{\mathrm{Europe}}(t) \text{ with T=45 days}$$

Outline

Large Variances for Estimators of Rare Event Probabilities

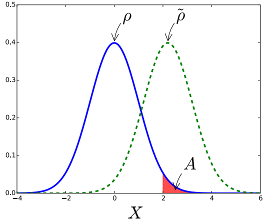
- Monte Carlo sampling of small probabilities (sampling the probability from iid random variables)

$$\gamma_A = \int \mathrm{d}x\, \rho(x) 1_A(x) = \mathbb{E}\left(1_A\right). \text{ Estimator: } \hat{\gamma}_A = \frac{1}{N}\sum_{n=1}^{N} 1_A(X_n).$$

- The variance of $\hat{\gamma}_A$ is $\mathrm{Var}\left(1_A\right)/N = \left(\gamma_A - \gamma_A^2\right)/N$. The relative error is
$$\mathrm{Er} \simeq \frac{1}{\sqrt{\gamma_A N}}.$$

- The number of observations has to grow at least as fast as the probability decreases to keep the relative error constant.

Importance Sampling



Tilted probability: $\rho(x) = L(x)\tilde{\rho}(x)$

- We sample a tilted probability with PDF $\tilde{\rho}(x)$.

$$\gamma_A = \int_A \rho(x)\,\mathrm{d}x = \int_A L(x)\tilde{\rho}(x)\,\mathrm{d}x. \text{ Estimator } \hat{\gamma}_A = \frac{1}{N}\sum_{n=1}^{N} L(X_n)\,1_A(X_n).$$

- If L is well chosen, rare events for ρ are common for $\tilde{\rho}$, and the variance is much lower.
- How to perform importance sampling for a climate model?

Donsker–Varadhan Large deviations for time averaged observables

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

$$P\left[\frac{1}{T}\int_0^T \langle Temp\rangle_{\mathrm{Europe}}\,\mathrm{d}t = a\right] \underset{T\to\infty}{\asymp} C\mathrm{e}^{-TI[a]}.$$

- $I(a)$ is the large deviation rate function. It has a minimum for the most probable value a_*, its second derivative at a_* describes the Gaussian fluctuations, but it describes also much rarer fluctuations.

Numerical Computation of Donsker–Varadhan Large Deviations

- Importance sampling: how to sample efficiently the tilted distribution

$$\tilde{P}_k\left(\{X(t)\}_{0\leq t\leq T}\right) = \frac{1}{\exp(T\lambda(k))} P_0\left(\{X(t)\}_{0\leq t\leq T}\right)\exp\left[k\int_0^T A(X(t))\,\mathrm{d}t\right] ?$$

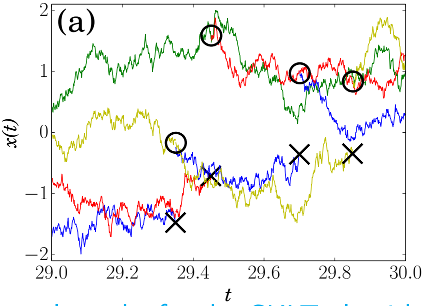
- We use the Giardina–Kurchan algorithm (Giardina et al 2006).
- We consider an ensemble of N trajectories $\{x_n(t)\}$. At each time $t_i = i\tau$, each trajectory may be killed or cloned according to the weights

$$\frac{1}{W_i(k)}\exp\left(k\int_{t_{i-1}}^{t_i} A(x_n(t))\,\mathrm{d}t\right) \text{ with } W_i(k) = \sum_{n=1}^{N}\exp\left(k\int_{t_{i-1}}^{t_i} A(x_n(t))\,\mathrm{d}t\right).$$

- For the mathematical aspects, see Del Moral's book (2004).

Genealogical Algorithm: Selecting and Cloning Trajectories

The trajectory statistics is tilted towards the events of interest.

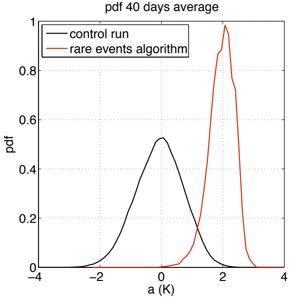


Sample paths for the GKLT algorithm

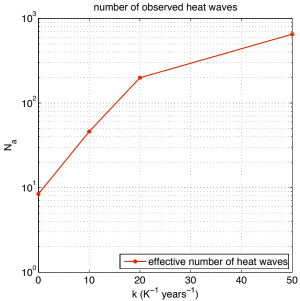
(from Bouchet, Jack, Lecomte, Nemoto, 2016)

- Computing numerically Donsker–Varadhan large deviations through a genealogical algorithm.

Importance Sampling of Extreme Heat Waves in a Climate Model



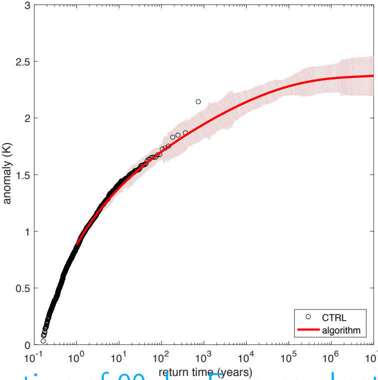
PDF of time averaged temperature



Heat wave number

- At a fixed numerical cost, we get hundreds more heat waves with the large deviation algorithm than with the control run.
- We can consider interesting dynamical studies.

The Return Times of Extreme Heat Waves



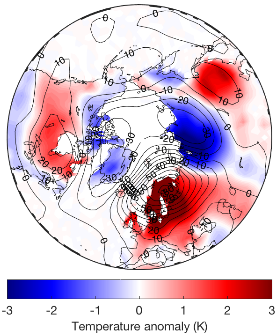
Return time of 90 day European heat waves

- At a fixed numerical cost, with the large deviation algorithm, we can study events which are several orders of magnitude rarer than the ones we could study with the control run.

A Typical Heat Wave

500 HPa geopotential height and temperature anomalies

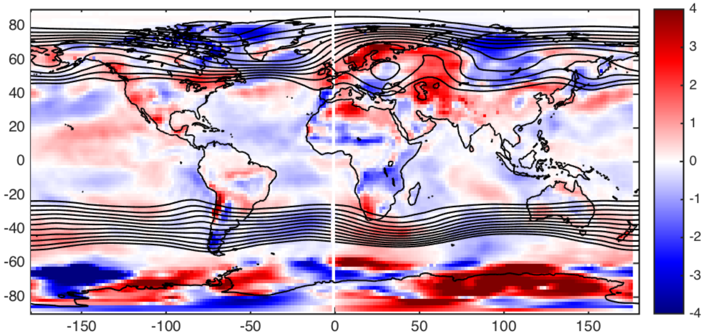
Heat Wave Conditional Statistics and Teleconnection Patterns



500 HPa geopotential height anomalies and temperature anomalies

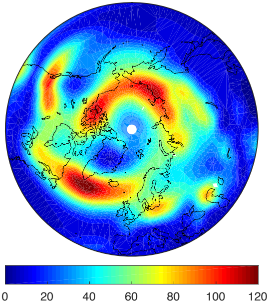
Heat wave statistics defined as statistics conditioned with $\frac{1}{T}\int_0^T \langle Temp \rangle_{\text{Europe}}(t)\,\mathrm{d}t > 2°\mathrm{C}$, with $T = 40\,\text{days}$.

The July 2018 Heat Wave(s)

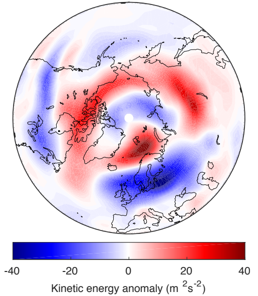


July 2018 observed (reanalysis) 500 HPa geopotential height and temperature anomalies (with respect to the last ten years).

Heat Waves and Shift of the Jet Stream



Northern hemisphere mean kinetic energy



Kinetic energy anomaly during the heat waves

- The European heat waves are associated with a northward shift of the jet stream over Europe and a southward shift over Asia.

Extreme Heat Waves: Conclusions

Conclusions:

- Large deviation algorithms provide a wonderful tool to sample rare events, for instance heat waves.
- It should open a new range of dynamical studies in GCM, even the more complex ones.

Work in progress:

- A dynamical study of heat waves based on hundreds of sampled heat waves.
- Relation with blocking events? Are they different types of dynamics leading to heats waves? Which physical processes? Relation between heat waves precursors and instantons?

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

Outline

Freidlin–Wentzell Theory

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

- Path integral representation of transition probabilities:

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

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

- 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)

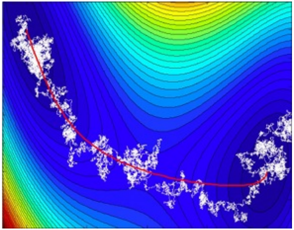


Figure by Eric Van den Eijnden

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

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

Transition Rates for Non-Gradient Dynamics

A non equilibrium Eyring–Kramers formula

$$\frac{d\mathbf{x}}{dt} = \mathbf{b}(\mathbf{x}) + \sqrt{2\varepsilon}\eta(t).$$

- We assume that there exists a transverse decomposition in the instanton neighborhood

$$\mathbf{b}(\mathbf{x}) = -\nabla V(\mathbf{x}) + \mathbf{G}(\mathbf{x}) \text{ with for all } \mathbf{x},\ \nabla V(\mathbf{x}).\mathbf{G}(\mathbf{x}) = 0.$$

- The transition rate then reads

$$\lambda \underset{\varepsilon\to 0}{\sim} \frac{|\lambda_*|}{2\pi}\sqrt{\frac{\det \mathrm{Hess}\, V(x_1)}{|\det \mathrm{Hess}\, V(x_*)|}} \exp\left(-\frac{\Delta V}{\varepsilon}\right) \exp\left\{-\int_{-\infty}^{+\infty} \mathrm{d}t\,[\nabla.G(X(t))]\right\},$$

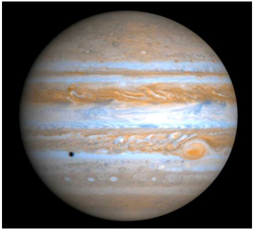
where λ_* is the negative eigenvalue corresponding to the unstable direction at the saddle point, for the dynamics (and not for V) and $\{X(t)\}$ is the instanton.

F. Bouchet and J. Reygner, Ann. Henri Poincaré, 2016.

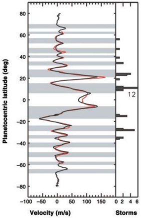
Outline

Jupiter's Zonal Jets

We look for a theoretical description of zonal jets



Jupiter's atmosphere



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

The Barotropic Quasi-Geostrophic Equations

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

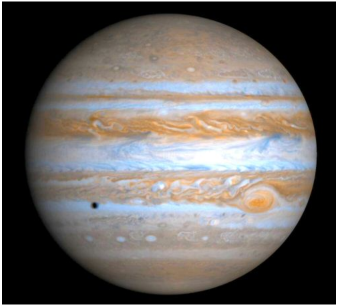
$$\frac{\partial q}{\partial t} + \mathbf{v}.\nabla q = \nu \Delta \omega - \alpha \omega + \sqrt{2\alpha} f_s,$$

  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.

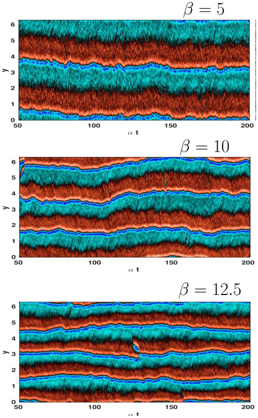
Dynamics of the Barotropic Quasi-Geostrophic Equations

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

Multistability for Quasi-Geostrophic Jets



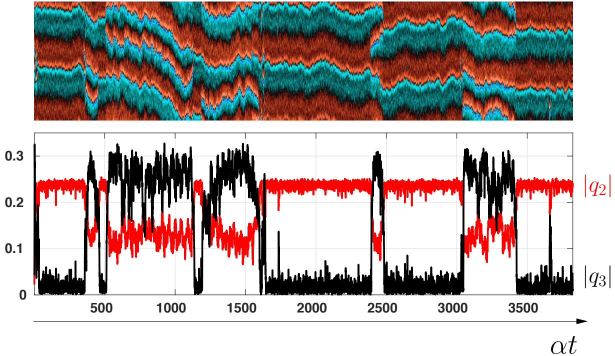
Jupiter's atmosphere



QG zonal turbulent jets

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

Rare Transitions Between Quasigeostrophic Jets



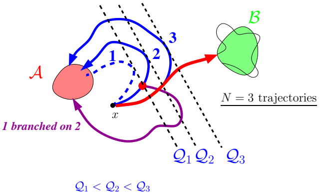
Rare transitions for quasigeostrophic jets (with E. Simonnet)

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

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.

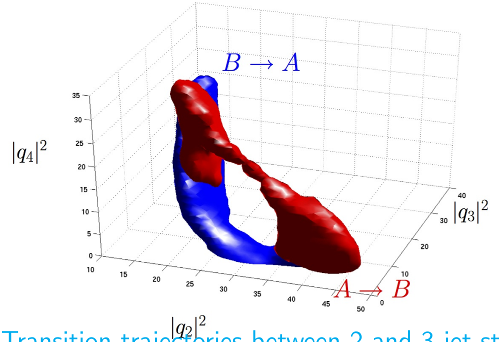
Cérou, Guyader (2007). Cérou, Guyader, Lelièvre, and Pommier (2011).

A Transition from 2 to 3 Jets

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

Atmosphere Jet "Instantons" Computed using the AMS

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

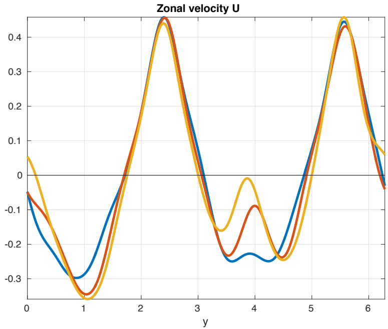


Transition trajectories between 2 and 3 jet states

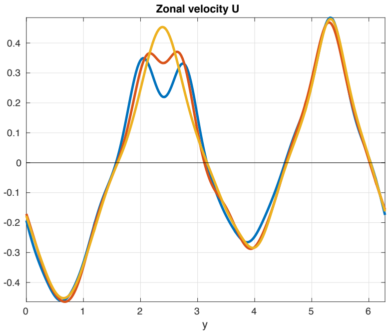
- The dynamics of turbulent transitions is predictible.
- Asymmetry between forward and backward transitions.

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

Evolution of Velocity Fields During the Transition



Nucleation of a new jet

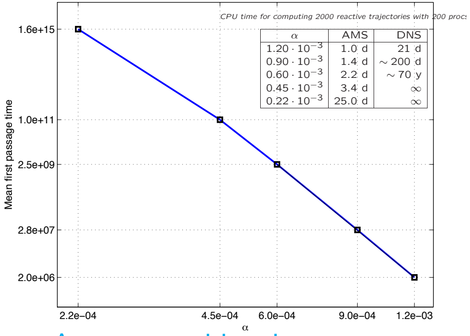


Merging of two jets

- Asymmetry between forward and backward transitions.

Transition Rates for Unreachable Regimes Through DNS

With the AMS we can estimate huge average transition times

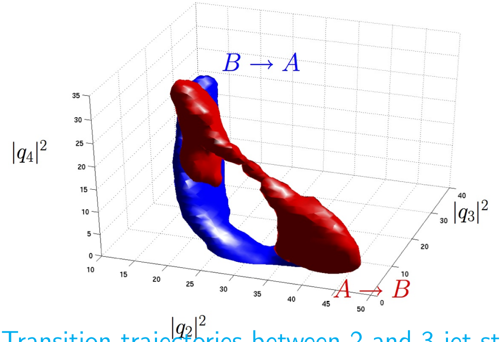


Average transition time versus α

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

Atmosphere Jet "Instantons" Computed using the AMS

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

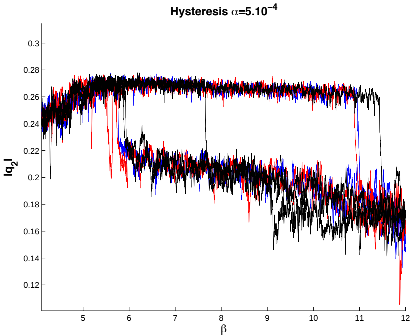


Transition trajectories between 2 and 3 jet states

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

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

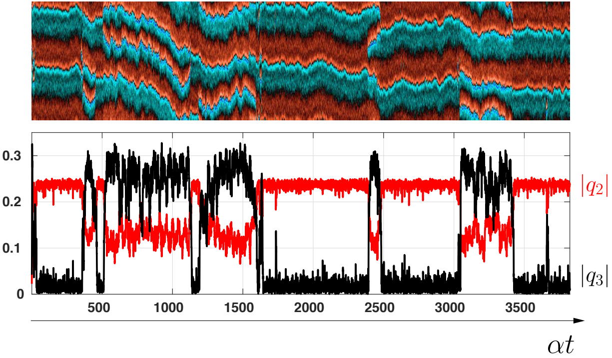
A Complex Internal Dynamics for the 3-Jet States



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

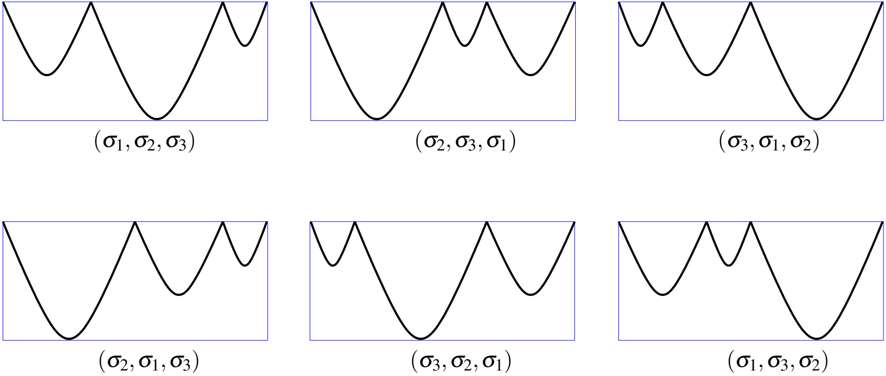


Rare transitions for quasigeostrophic jets

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

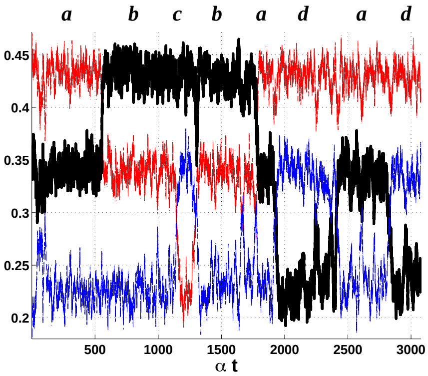
A Family of Different 3-Jet Attractors

Symmetry breaking within the set of 3-jet attractors



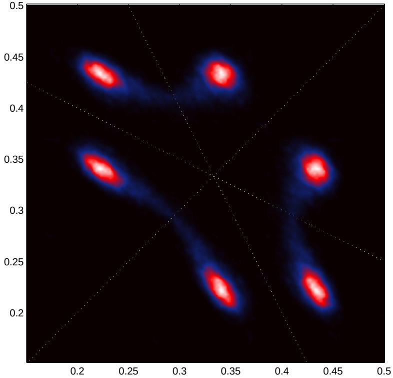
Schematic zonal velocity fields $U(y)$ for the 3-jet attractors

Internal Multistability for the 3-Jet Attractors



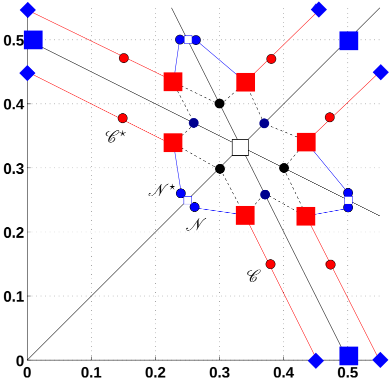
Timeseries for the distance between jets within the 3-jet attractors

Internal Multistability for the 3-Jet Attractors



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

Bifurcation Diagram for the 3-Jet Attractors

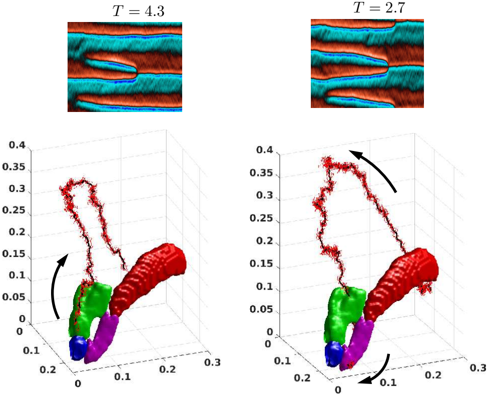


Attractors and saddles for the 3 jet states

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

A Richer Transition Phenomenology

Transitions through states with four jets are possible



Abrupt Changes for Atmosphere Jets: Conclusions

- For the first time we observe the Freidlin-Wentzell phenomenology (instantons, transition rates, and so on) for rare transitions of turbulent flows.
- This is analogous to Jupiter's abrupt climate change.
- We can sample the ultra rare transitions using a rare event algorithm.
- This should have an impact on future studies of abrupt climate changes.

Collaborators

- Sampling extreme heat waves using large deviation algorithms (with J. Wouters and F. Ragone).
- Numerical simulation of abrupt transitions for Jupiter zonal jets using Adaptive Multilevel Splitting algorithms (with J. Rolland and E. Simonnet).