Extreme Events in Weather and Climate
CriticalEarth Meeting, Nijmegen NL
April 29, 2022

Extreme Events in Complex Systems via Large Deviation Theory

Tobias Grafke

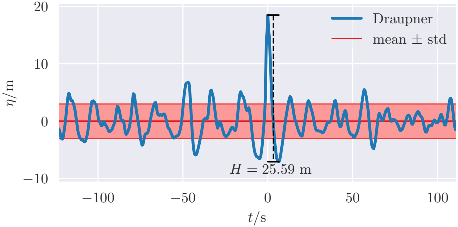
Rogue waves:

Events of extreme ocean surface elevation.

- Mechanism not fully understood
- Probably caused by **nonlinear amplification** (*modulational instability*) out of a background of (smaller) waves
- Probability density function unknown.

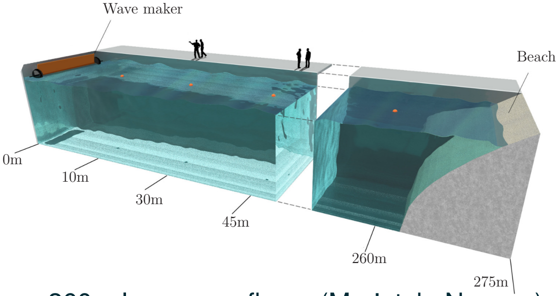
Goal: Estimate **tails** of the distribution

Tanker "Stolt Surf" in 1977, New York Times



"Draupner Wave", Jan 1, 1995

Experimental Setup



- 260m long wave flume (Marintek, Norway)
- Wave maker generates **random signal**
- Planar wave **propagates** along the flume
- 19 probes record **elevation signal** $\eta(t)$

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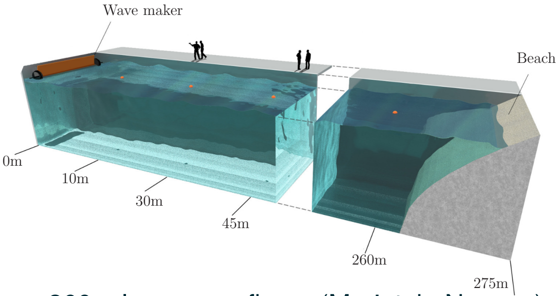

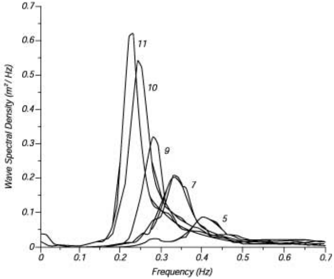

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Input signal: JONSWAP observational spectrum

Defined by 2 Parameters:

- H_s: sign. wave height
- BFI: degree of nonlinearity

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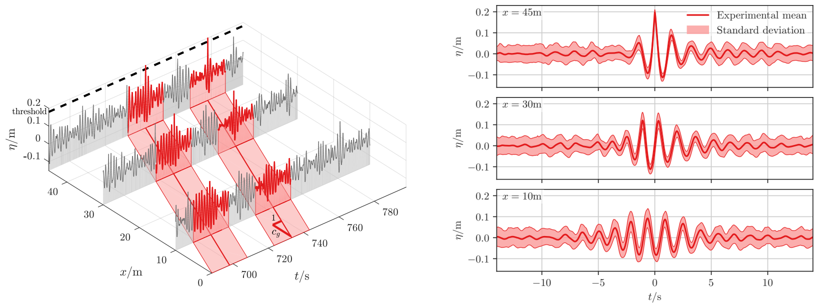
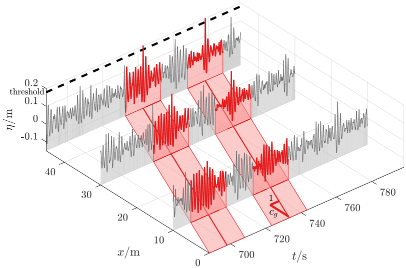
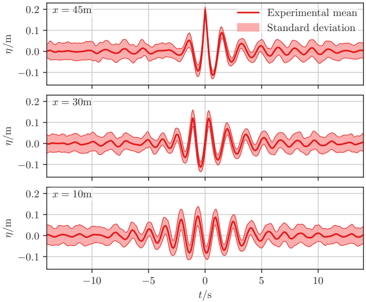
Extreme Event Filtering



- At fixed location x along flume, measure events that exceed threshold z
- Track wave packet backwards in space, using c_g
- Build collection of extreme event precursors
- Compute average extreme event and fluctuations





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Claim: Rogue Waves can be described via **Large Deviations**

Large Deviations in Random Dynamical Systems

Consider **dynamical system** $x \in \Omega$, with **random parameters** and **random initial conditions**,

$$\dot{x} = b(x,\theta)\,, \;\; x(t{=}0) = x_0(\theta), \;\; \theta \sim \mu(\theta)$$

and some **observable** $f : \Omega \mapsto \mathbb{R}$, then

$$P_T(z) = \mathcal{P}(f(x(T)) \geq z) = \mu(\Omega(z))$$

where $\Omega(z) = \{\theta \in \Omega \mid f(x(T;\theta)) \geq z\}$.

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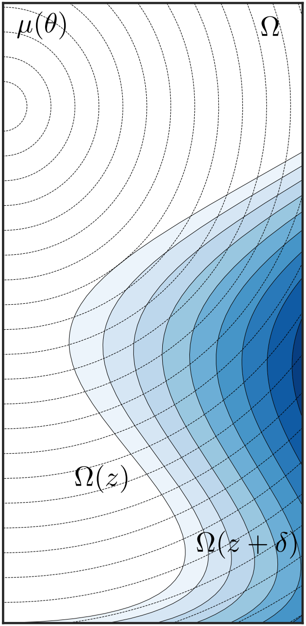
Ω: Space of random parameters θ

μ: Random measure of θ on Ω

$\Omega(z)$: Subset of parameters that exceed threshold z under evolution



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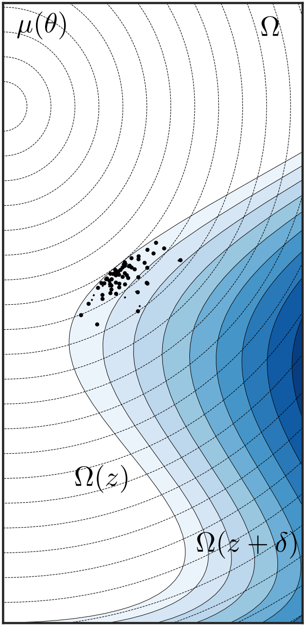

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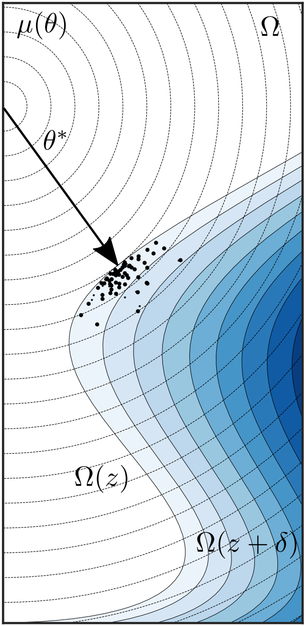

Intuition

We can replace the **integral over** $\Omega(z)$ by its **most likely point** (dominating point, instanton) $\theta^*(z)$, i.e. the most likely random parameters that still lead to the rare event.

This transforms a **difficult sampling problem** into an **constrained optimization problem**

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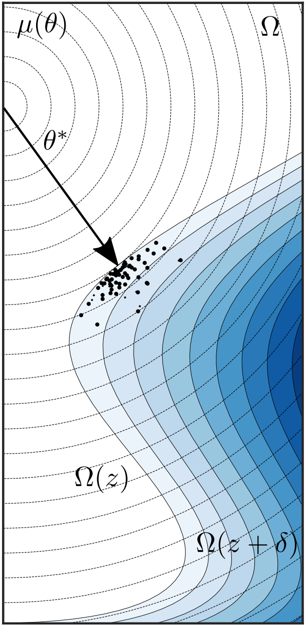
Then **large deviation principle** (LDP) says

$$P_T(z) \asymp \exp\left(-\min_{\theta\in\Omega(z)} I(\theta)\right)$$

with rate function $I(\theta) = \max_\eta \{\langle \eta, \theta\rangle - S(\eta)\}$ and cumulant generating function $S(\eta) = \log \mathbb{E} e^{\langle \eta, \theta\rangle}$

Dominated for $z \to \infty$ by **instanton** or **minimizer**

$$\theta^*(z) = \operatorname*{argmin}_{\theta\in\Omega(z)} I(\theta)$$



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Evolution of a narrow-banded, uni-directional **wave envelope** $\psi(t,x)$ on the surface of a fluid with **infinite depth**:

nonlinear Schrödinger equation (NLS)

$$\partial_x \psi + 2\tfrac{k_0}{\omega_0}\partial_t\psi + i\tfrac{k_0}{\omega_0^2}\partial_t^2\psi + 2ik_0^3|\psi|^2\psi = 0\,,\quad \psi(x=0)=\psi_0$$

on domain $t\in\Omega$ with **surface elevation** $\eta(t,x)=\mathrm{Re}(\psi(t,x)e^{i(k_0x-\omega_0 t)})$

Rogue waves in MNLS

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Instanton computation

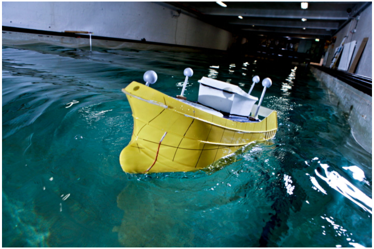
We have the above LDT for

$$\begin{cases} b(\psi) = \text{NLS} \\ \psi_0 \sim \mu = \text{JONSWAP} \\ f(\psi(L)) = \max_{t\in\Omega} |\psi(X,t)| \end{cases}$$

and find numerically

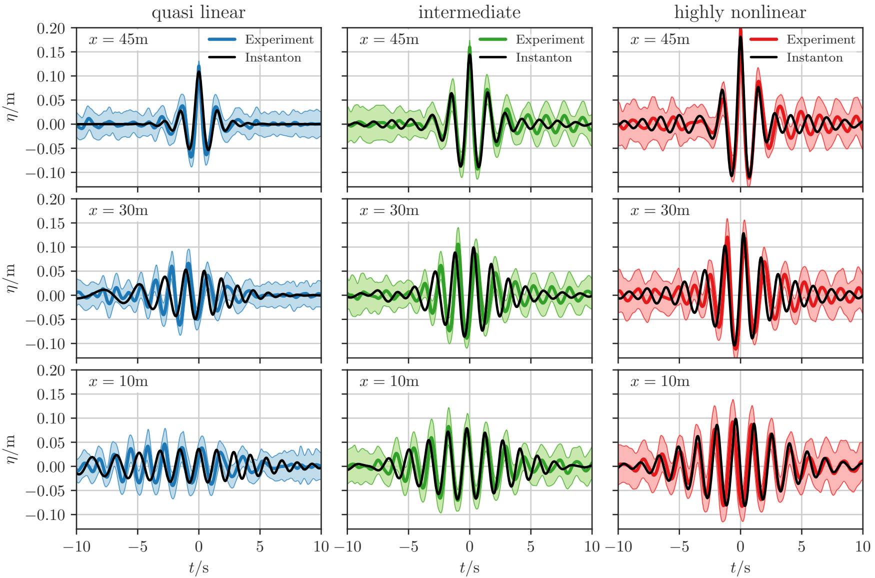
$$P(z) = \mathcal{P}(f(\psi(L)) > z) \sim \exp(-S(\psi_0^*))$$

by computing instanton ψ^*.



Compare ψ^* to experiment!

Comparison: Experiment vs Instanton



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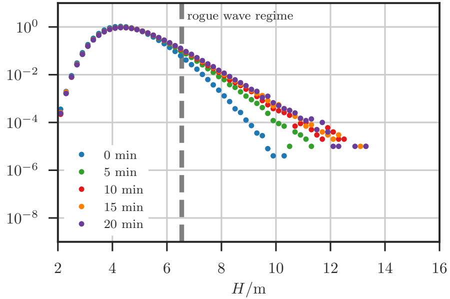
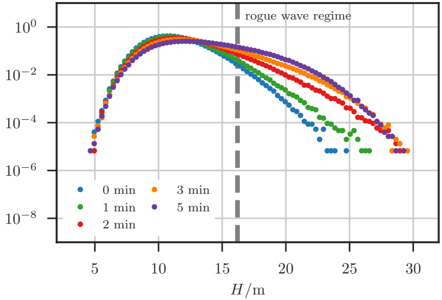
Probabilities

rough sea ($H_s = 3.3$m, BFI $= 0.34$)



high sea ($H_s = 8.2$m, BFI $= 0.85$)



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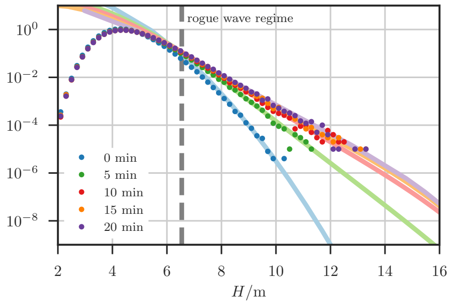

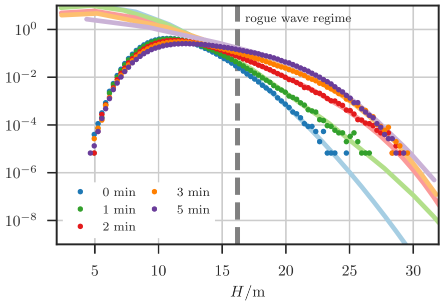

Comparison between **Monte Carlo** (dots) and **LDT** (lines):

LDT is able to **predict tails** of **rogue wave** distribution.

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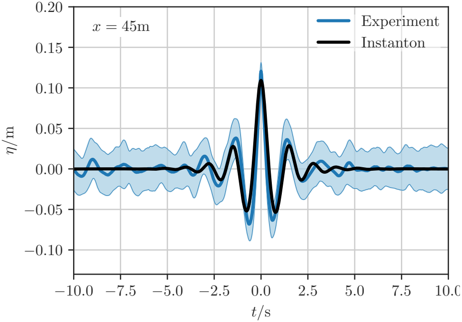
Summary

- Experimental evidence of **hydrodynamic instanton**
- Each **Rogue Wave** event in **Wave Flume** experiment closely resembles **Instanton** solution
- Contains **linear theory** as limiting case
- Contains **Peregrine soliton** in nonlinear limit
- Offers **unified description** of Rogue waves



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The way rare events occur is often predictable — it is dominated by the *least unlikely* scenario — which is the essence of LDT

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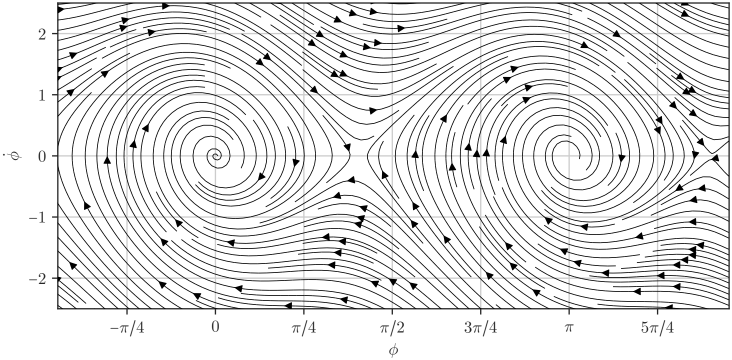

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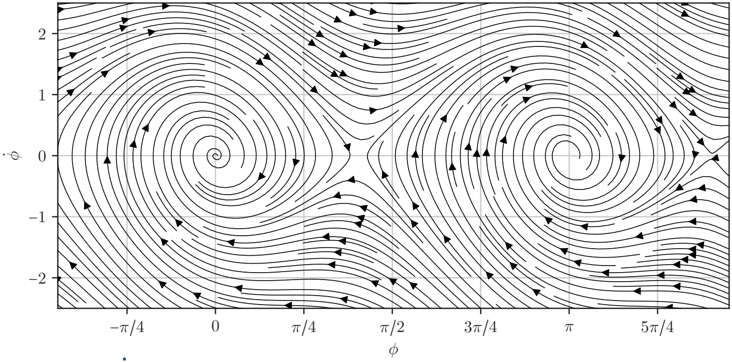

$$
\begin{aligned}
d\phi &= \dot\phi\, dt + \sigma\, dW_1, \\
d\dot\phi &= -V'(\phi)\, dt - \gamma\dot\phi\, dt + \sigma\, dW_2
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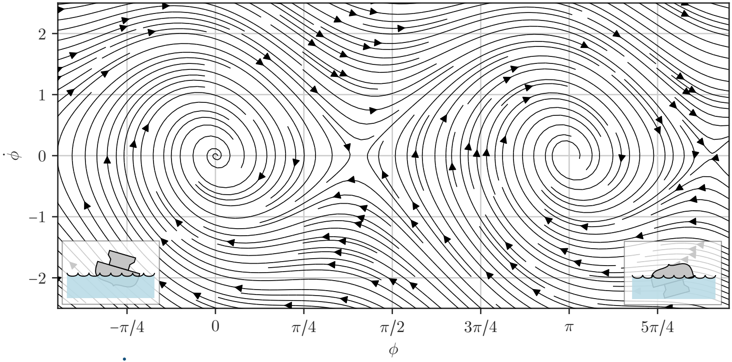

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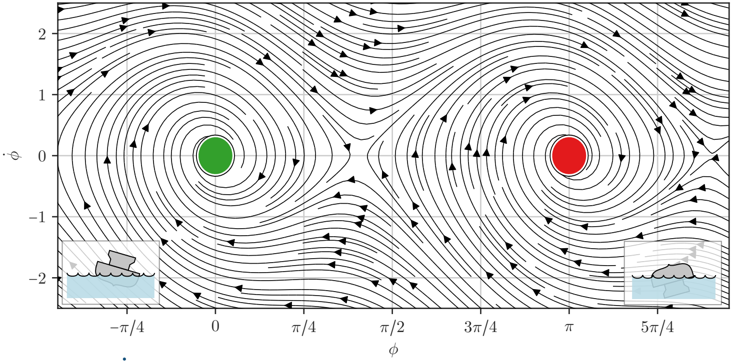

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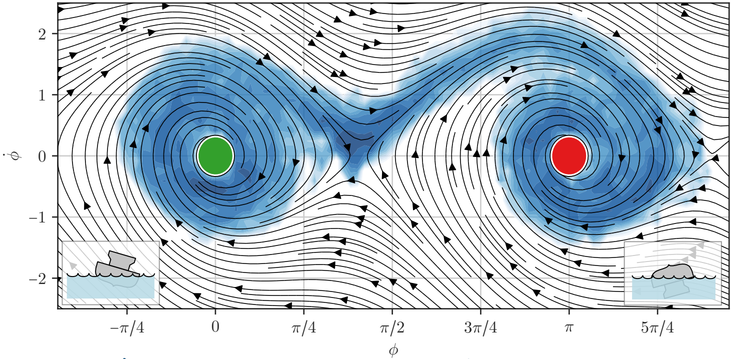

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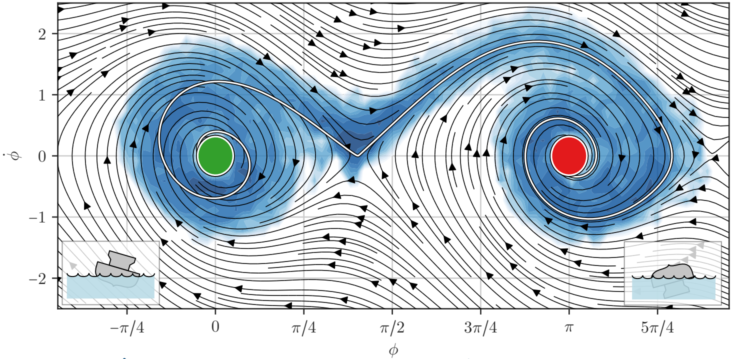

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Large deviation theory for stochastic processes

A family of stochastic processes $\{X_t^\varepsilon\}_{t\in[0,T]}$ with smallness-parameter ε (e.g. $\varepsilon = 1/N$, or $\varepsilon = k_B T$, etc) fulfills **large deviation principle**:

The probability that $\{X^\varepsilon(t)\}_{t\in[0,T]}$ is close to a path $\{\phi(t)\}_{t\in[0,T]}$ is

$$\forall\,\delta > 0 \qquad \mathcal{P}^\varepsilon\left\{\sup_{0\le t\le T} |X^\varepsilon(t) - \phi(t)| < \delta\right\} \asymp \exp\left(-\varepsilon^{-1} S_T(\phi)\right) \text{ for } \varepsilon \to 0$$

where $S_T(\phi)$ is the **rate function** or **action**.

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The probability of **transition** from x to y is reduced to a **minimization** problem

$$\mathcal{P}^\varepsilon\left\{X^\varepsilon(T)\in\mathcal{B}_\delta(y)|X^\varepsilon(0)=x\right\} \asymp \exp\left(-\varepsilon^{-1}\inf_{\phi:\phi(0)=x,\phi(T)=y} S_T(\phi)\right)$$

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Here, $\asymp$ is log-asymptotic equivalence, i.e.

$$\lim_{\varepsilon\to 0} \varepsilon \log \mathcal{P}^\varepsilon = -\inf_{\phi\in\mathscr{C}_x^y} S_T(\phi) \text{ with e.g. } \mathscr{C}_x^y = \{\phi \mid \phi(0) = x, \phi(T) = y\}$$

We also call the **minimizer** $\phi^*(t) = \operatorname*{argmin}_{\phi\in\mathscr{C}_x^y} S_T(\phi)$ the **instanton**

In particular consider SDE (diffusion) for $X_t^\varepsilon \in \mathbb{R}^n$,

$$dX_t^\varepsilon = b(X_t^\varepsilon)\,dt + \sqrt{\varepsilon}\sigma dW_t\,,$$

with "drift" $b : \mathbb{R}^n \to \mathbb{R}^n$ and "noise" with covariance $\chi = \sigma\sigma^T$, we have

$$S_T(\phi) = \tfrac{1}{2}\int_0^T |\dot\phi - b(\phi)|_\chi^2\,dt = \int_0^T L(\phi,\dot\phi)\,dt\,,$$

for **Lagrangian** $L(\phi,\dot\phi)$ (follows by contraction from Schilder's theorem).

We are interested in

$$\phi^* = \operatorname*{argmin}_{\phi\in\mathscr{C}} \int_0^T L(\phi,\dot\phi)\,dt$$

which is the **maximum likelihood pathway** or **instanton**, which fulfills the corresponding Hamilton's equations ($H(\phi,\theta) = \min_{\dot\phi}\{\dot\phi\cdot\theta - L(\phi,\dot\phi)\}$):

$$\begin{cases}\dot\phi &= b(\phi) + \chi\theta\\ \dot\theta &= (-\nabla b)^\top\theta\end{cases}$$ with appropriate boundary conditions.

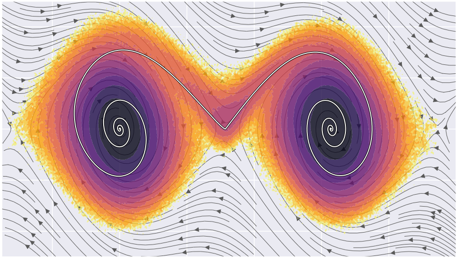
Mark I Freidlin and Alexander D Wentzell. Vol. 260. Springer, 2012

Main Problem

Find the **instanton** ϕ^* such that

$$S_T(\phi^*) = \inf_{\phi \in \mathscr{C}_x^y} S_T(\phi)$$

where $\mathscr{C}_x^y$ is the set of trajectories that transition $x \to y$



Knowledge of the optimal trajectory gives us

1. **Probability** of event, $\mathcal{P} \sim \exp\left(-\varepsilon^{-1} S_T(\phi^*)\right)$
2. Most likely **occurrence**, ϕ^* itself (allows for prediction, exploring causes, etc.)
3. Most effective way to force event (optimal control), **optimal fluctuation**

Ornstein-Uhlenbeck process

$$du = -\gamma u \, dt + \sqrt{\varepsilon} \, dW \,, \quad \gamma > 0 \,.$$

Consider events with $u(T) \geq z$

The **instanton** is

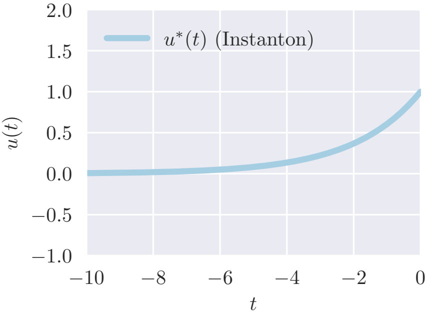
$$u^*(t) = z e^{\gamma(t-T)} \left(\frac{1 - e^{-2\gamma t}}{1 - e^{-2\gamma T}} \right) \,,$$

obtained from **constrained optimization**

$$\inf_{\{u_t\} \in \mathscr{C}_0^z} \mathcal{S}_T(u) = \inf_{\{u_t\} \in \mathscr{C}_0^z} \tfrac{1}{2} \int_0^T |\dot{u} + \gamma u|^2 \, dt$$

over the set

$$\mathscr{C}_0^z = \left\{ \{u_t\} \,\middle|\, u(0) = 0, u(T) = z \right\}$$



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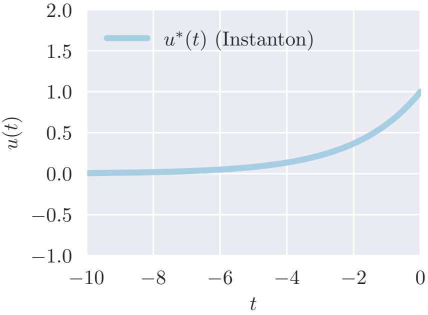
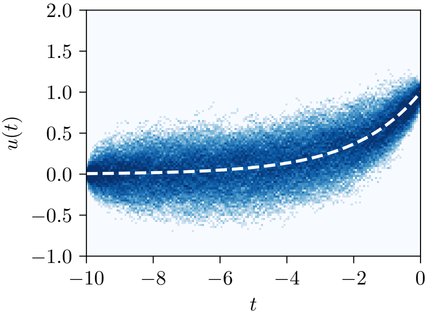




Example: Ornstein-Uhlenbeck

Ornstein-Uhlenbeck process

$$du = -\gamma u\, dt + \sqrt{\varepsilon}\, dW\,, \quad \gamma > 0\,.$$

Consider events with $u(T) \geq z$

The **instanton** is

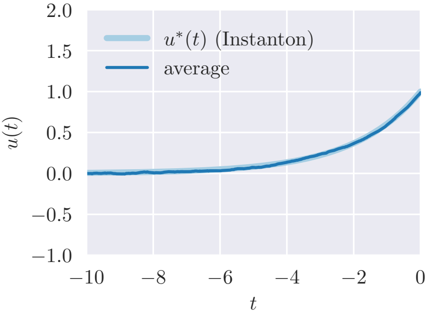
$$u^*(t) = z e^{\gamma(t-T)} \left(\frac{1 - e^{-2\gamma t}}{1 - e^{-2\gamma T}}\right)\,,$$

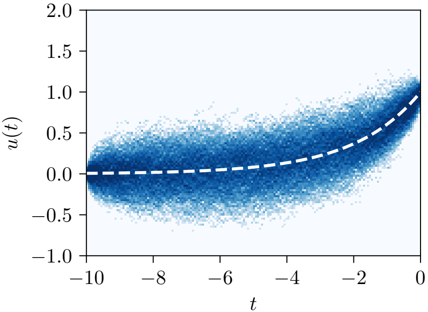
obtained from **constrained optimization**

$$\inf_{\{u_t\}\in\mathscr{C}_0^z} \mathcal{S}_T(u) = \inf_{\{u_t\}\in\mathscr{C}_0^z} \tfrac{1}{2}\int_0^T |\dot u + \gamma u|^2\, dt$$

over the set

$$\mathscr{C}_0^z = \Big\{\{u_t\}\ \Big|\ u(0) = 0, u(T) = z\Big\}$$





3D **Navier-Stokes** equation

$$\begin{cases} \partial_t u + u \cdot \nabla u = -\nabla p + \Delta u + \sqrt{\varepsilon}\eta \,, \\ \nabla \cdot u = 0 \,, \\ \mathbb{E}\left(\eta(x,t)\eta(x',t')\right) = \chi(x-x')\delta(t-t') \,. \end{cases}$$

We want to find the **most likely** extreme event that realizes an extreme **vorticity** or **strain**:

$$\omega_z(0,0) \geq a \qquad \text{or} \qquad \partial_z u_z(0,0) \geq a \,.$$

The corresponding **instanton** is the solution of the equations

$$\begin{cases} \partial_t u_{\mathrm{I}} + \mathbb{P}\left[(u_{\mathrm{I}} \cdot \nabla) u_{\mathrm{I}}\right] - \Delta u_{\mathrm{I}} = \chi * p_{\mathrm{I}} \,, \\ \partial_t p_{\mathrm{I}} + \mathbb{P}\left[(u_{\mathrm{I}} \cdot \nabla) p_{\mathrm{I}} + (\nabla p_{\mathrm{I}})^\top u_{\mathrm{I}}\right] + \Delta p_{\mathrm{I}} = 0 \,, \end{cases}$$

(for the Leray-projector $\mathbb{P} = \mathrm{Id} - \nabla \Delta^{-1} \nabla \cdot$)

Observable: **Vorticity**

$$\omega_z \geq a$$

Compare **conditional average** from stochastic DNS against **instanton** from optimization problem.

This is a **large** problem ($\approx 128^3 \times 1000$ dofs).

Instantons for the 3D Navier-Stokes equation

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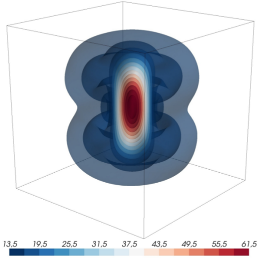
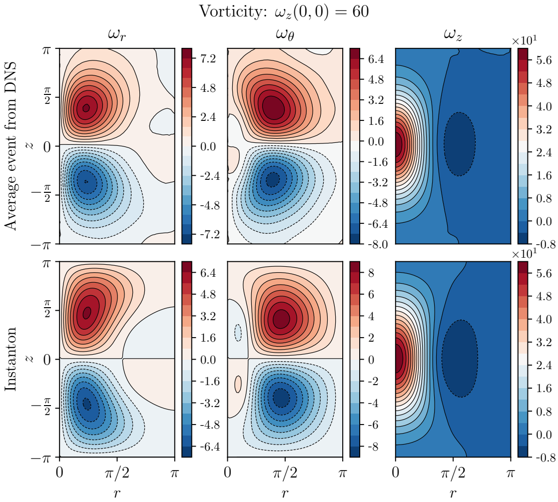


$$\omega_z(0,0) = 75.0$$



Observable: **Strain**

$$\partial_z u_z \geq a$$

Spontaneous Symmetry Breaking

While the **observable** is symmetric, and the **action** is symmetric, the **minimizer** need not be symmetric.

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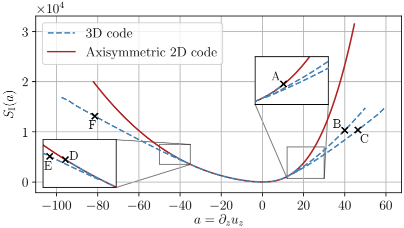
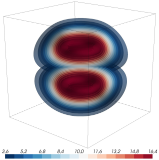
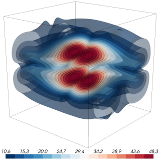
Small strains are rotationally symmetric.

For large positive or negative straing values, symmetry is broken!

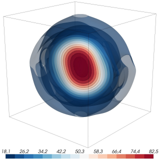




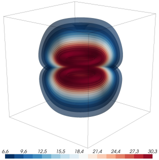
A: $\partial_z u_z(0,0) = 19.0$



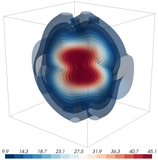
B: $\partial_z u_z(0,0) = 40.0$



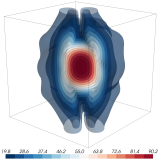
C: $\partial_z u_z(0,0) = 46.4$



D: $\partial_z u_z(0,0) = -45.4$



E: $\partial_z u_z(0,0) = -48.5$



F: $\partial_z u_z(0,0) = -81.4$

Observable: **Strain**

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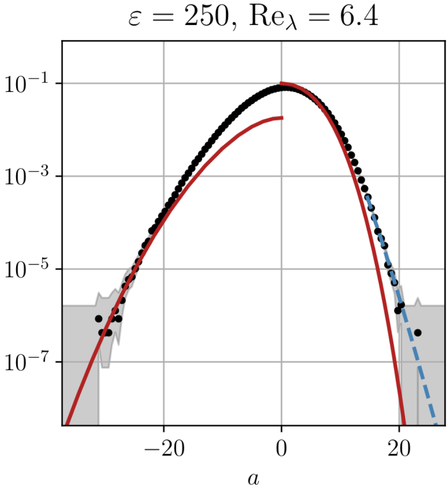
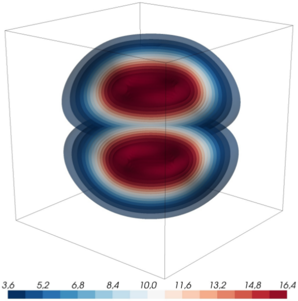


Large Deviation Theory

- Rare events can effectively be treated by **large deviation theory**
- This applies both to **random parameters** and **random noise**, and even **random fields**
- Yields **most likely configuration** that realizes a rare event
- Yields **probability scaling** for rare events



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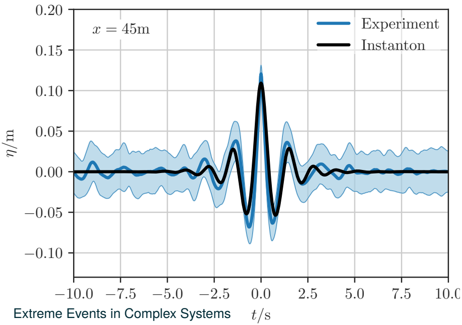

Timo Schorlepp, Tobias Grafke, Sandra May, and Rainer Grauer. In: *arXiv:2107.06153 [physics]* (July 2021)
Tobias Grafke and Eric Vanden-Eijnden. In: *Chaos: An Interdisciplinary Journal of Nonlinear Science* 29.6 (June 2019). DOI: 10.1063/1.5084025

Problem

Large Deviations captures only the **exponential scaling**:

$$\mathcal{P}(z) \sim \exp(-\varepsilon^{-1} S(\phi_z^*)) \quad \to \quad P(z) = \underbrace{C(z)}_{!!!} \exp(-\varepsilon^{-1} S(\phi_z^*))$$

but constant (**prefactor**) unknown!

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Laplace Method: For some $S : \Omega \mapsto \mathbb{R}$ with unique minimum x^*, we have

$$\int_\Omega \exp(-\varepsilon^{-1} S(x))\, dx \ \xrightarrow{\varepsilon \to 0}\ (2\pi\varepsilon)^{d/2} \det(\nabla\nabla S(x^*))^{-1/2} \exp(-\varepsilon^{-1} S(x^*))$$

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(1) Find **Large Deviation Minimizer**

(2) Find **determinant** of the **second variation** of the action

(in general, this will be a functional determinant)

Computation of the Fluctuation Determinant

This amounts to accounting for the **effects of fluctuations** ξ around the minimizer ϕ_z^*.

Perform the change of measure from X_t^ε to

$$\xi_t = \varepsilon^{-1/2} \left(X_t^\varepsilon - \phi_z^* \right) \, .$$

Expanding change-of-measure in ε yields

$\mathcal{O}(e^{\varepsilon^{-1}})$ is the LDT contribution

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The **prefactor** contribution is then available as expectation over the **fluctuation process**

$$d\xi_t = \nabla b(\phi_z^*)\, \xi_t \, dt + \sigma dW_t$$

via

$$C(z) = \mathbb{E}_\xi \exp \left(\frac{1}{2} \int_0^T \nabla\nabla \langle b(\phi_z^*), \theta \rangle : \xi_t \xi_t \, dt \right)$$

As we will see next, the effect of these fluctuations can be accounted for exactly!

Computation of the Fluctuation Determinant

For $dX_t^\varepsilon = b(X_t^\varepsilon)\,dt + \sqrt{\varepsilon}\sigma dW_t$, with $\chi = \sigma\sigma^\top$, the prefactor $C(z)$ can be calculated via a **Riccati equation** for $Q : [0,T] \mapsto \mathbb{R}^{d\times d}$

$$\dot{Q} = Q\nabla\nabla\langle b(\phi), \theta\rangle Q + Q(\nabla b(\phi))^\top + (\nabla b(\phi))Q + \chi$$

which is related to the covariance of the **fluctuations** around the minimizer.

$$C(z) = \sqrt{\frac{\varepsilon\kappa}{2\pi}}\,\langle\theta(T), Q(T)\theta(T)\rangle^{-1/2}\,\exp\Big(-\tfrac{1}{2}\int_0^T \mathrm{tr}[\nabla\nabla\langle b(\phi),\theta\rangle Q]\,dt\Big)$$

(where (ϕ, θ) is the minimizer and its conjugate momentum, and κ is a curvature term).

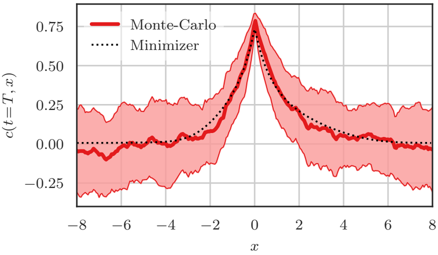
In QFT this is called the **fluctuation determinant** on the **instanton background**.

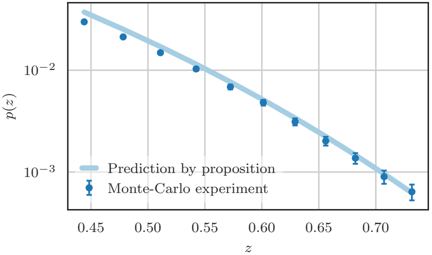
Timo Schorlepp, Tobias Grafke, and Rainer Grauer. In: *Journal of Physics A: Mathematical and Theoretical* (Apr. 2021). DOI: 10.1088/1751-8121/abfb26

Tobias Grafke, Tobias Schäfer, and Eric Vanden-Eijnden. In: *arXiv:2103.04837* (Apr. 2021)

Freddy Bouchet and Julien Reygner. In: *arXiv:2108.06916 [cond-mat]* (Aug. 2021)

Example: Stochastic Advection-Diffusion-Reaction equation





For advection-diffusion-reaction equation

$$\partial_t c = \kappa \partial_x^2 c - v(x)\partial_x c - \alpha c - \gamma c^3 + \sqrt{2\varepsilon}\eta\,,$$

We are interested in the probability that a sample exceeds the threshold z at the location $x = 0$ at time $t = T$, i.e.

$$p(z) = \mathcal{P}\big(c(x{=}0, t{=}T) \geq z\big)\,.$$

Summary

- We can reason about path-space measures via **sample path large deviations**
- This allows us to compute limiting **probabilities**, **expectations**, **hitting times**, etc in some limit (such as small noise)
- Sharp estimates are obtained via computation of **fluctuation determinant**
- This is applicable to many systems of relevance

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Tobias Grafke, Rainer Grauer, and Tobias Schäfer. In: *Journal of Physics A: Mathematical and Theoretical* 48.33 (Aug. 2015). DOI: 10.1088/1751-8113/48/33/333001