WCPM/CSC Seminar
University of Warwick
30 Apr, 2018

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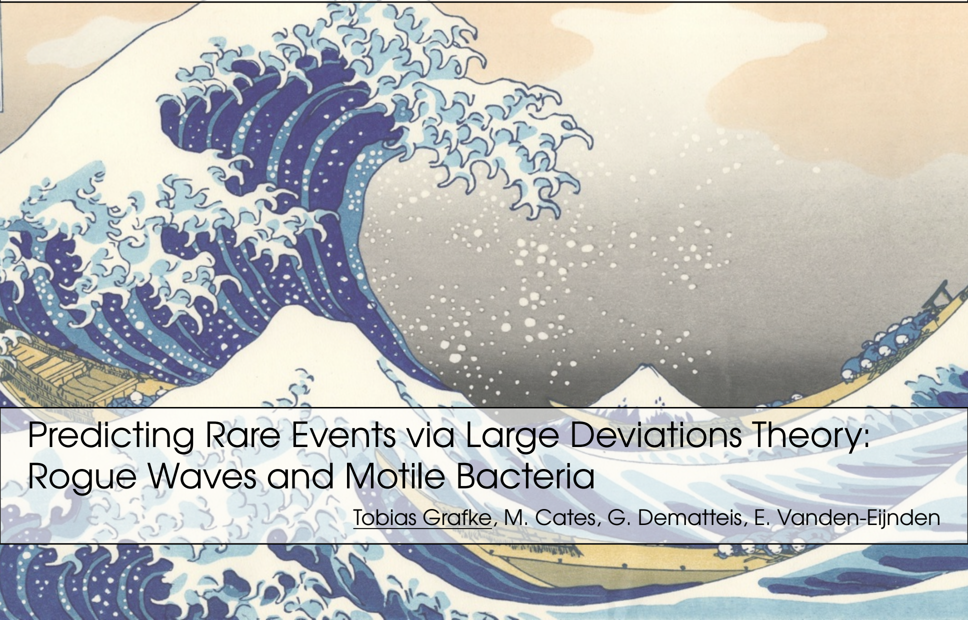

Predicting Rare Events via Large Deviations Theory: Rogue Waves and Motile Bacteria

Tobias Grafke, M. Cates, G. Dematteis, E. Vanden-Eijnden

Rare events matter

- Rare events are important if they are **extreme**
- Or **separation of scales** makes them common after all
- underlying dynamics might be **very complex**, and analytical solutions are not available in most cases: Turbulence, Climate, chemical- or biological systems
- Direct numerical simulations (sampling) is **infeasible** because events are very rare
- Rare events are often **predictable**: Requires computational approaches based on LDT

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- Calculation of the least unlikely scenario (maximum likelihood pathway, MLP) reduces to a deterministic optimization problem

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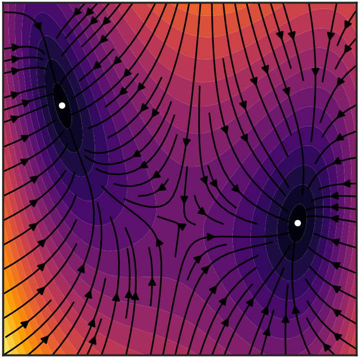

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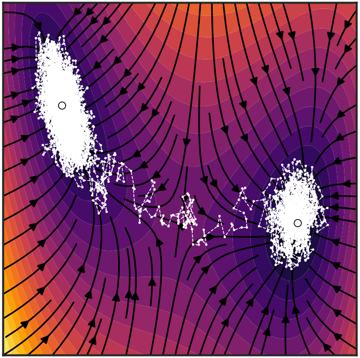

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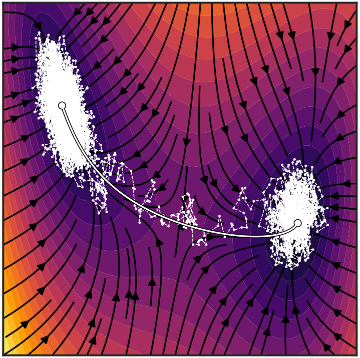

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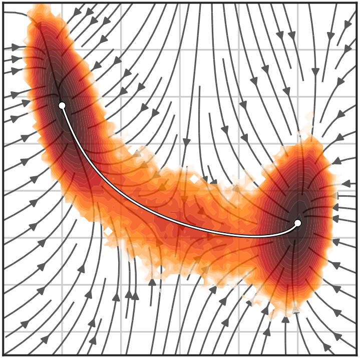

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A family of stochastic processes $\{X_t^\varepsilon\}_{t\in[0,T]}$ with smallness-parameter ε (e.g. $\varepsilon = 1/N$, or $\varepsilon = k_B T$, etc) fulfils **large deviation principle**:

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

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

where $\mathcal{I}_T(\phi)$ is the **rate function**.

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The probability of **hitting** set $A_z = \{x|F(x)=z\}$ is reduced to a **minimisation** problem

$$\mathcal{P}^\varepsilon\left\{X^\varepsilon(T)\in A_z|X^\varepsilon(0)=x\right\}\asymp\exp\left(-\varepsilon^{-1}\inf_{\phi:\phi(0)=x,F(\phi(T))=z}\mathcal{I}_T(\phi)\right)$$

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

$$\lim_{\epsilon\to 0}\varepsilon\log\mathcal{P}^\varepsilon=-\inf_{\phi\in\mathscr{C}}I_T(\phi)\text{ with e.g. }\mathscr{C}=\left\{\{x\}_{t\in[0,T]}|x(0)=x,F(x(T))=z\right\}$$

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

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

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 likelyhood pathway** (MLP).

Physicists approach: Path integral formalism

Consider

$$\dot{x} = b(x) + \eta$$

with white noise η with covariance

$$\langle \eta_i(t)\eta_j(t')\rangle = \epsilon\chi_{ij}\delta(t-t')$$

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but $x = x[\eta]$, with $\eta = \dot{x} - b(x)$, so that (ignoring Jacobian)

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$$\frac{\delta I}{\delta \phi^*} = 0,$$ (**Instanton**, semi-classical trajectory)

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Rate function $\leftrightarrow$ Action, MLP $\leftrightarrow$ Instanton, LDP $\leftrightarrow$ Hamiltonian principle

Main problem

Find the **maximum likelyhood pathway** (MLP) ϕ^* realizing an event, i.e. such that

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Maximum likelyhood pathway and rare events

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Knowledge of the optimal trajectory gives us

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

Ornstein-Uhlenbeck process

$$du = b(u)\,dt + dW\,, \quad b(u) = -\gamma u\,, \quad \gamma > 0$$

Consider extreme events with $u(T) = z$ (so $F(u) = u(T)$).

The **instanton** is

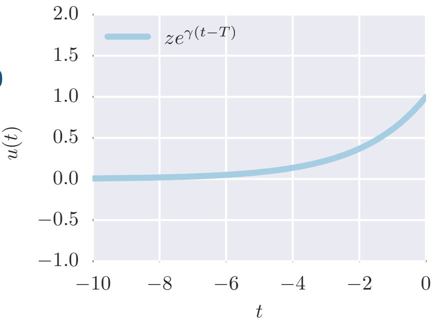
$$u^*(t) = ze^{\gamma(t-T)}\left(\frac{1-e^{-2\gamma t}}{1-e^{-2\gamma T}}\right),$$

obtained from **constrained optimization**

$$\inf_{\{u_t\}\in\mathcal{U}_z} \mathcal{I}_T(z) = \inf_{\{u_t\}\in\mathcal{U}_z} \tfrac{1}{2}\int_0^T |\dot u + \gamma u|^2\,dt$$

over the set

$$\mathcal{U}_z = \left\{\{u_t\}\;\middle|\; F(u_T) = z\right\}$$



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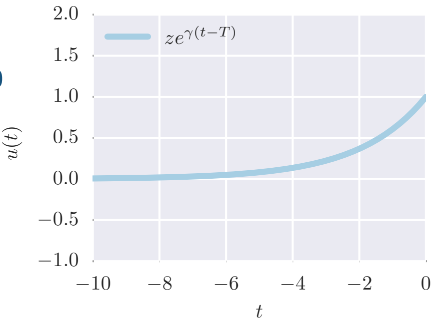

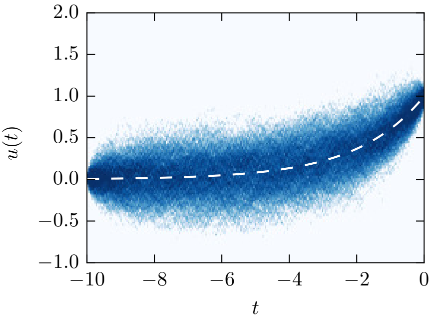

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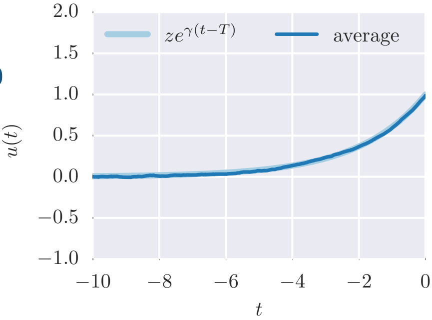

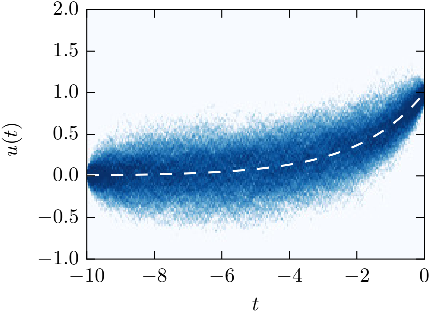

Special case: Systems in **detailed balance**. For example,

$$dX_t^\epsilon = -\nabla U(X_t^\epsilon)\, dt + \sqrt{2\epsilon}\, dW_t$$

Then

$$I_T(\phi) = \tfrac{1}{4}\int_0^T |\dot\phi + \nabla U|^2\, dt$$

is minimized either by $\dot\phi = -\nabla U$ (“sliding” down-hill) or

$$\begin{aligned} I_T(\phi) = \tfrac{1}{4}\int_0^T |\dot\phi + \nabla U|^2\, dt &= \tfrac{1}{4}\int_0^T |\dot\phi - \nabla U|^2\, dt + \int_0^T \nabla U \cdot \dot\phi\, dt \\ &= U(\phi_{\text{end}}) - U(\phi_{\text{start}}) \qquad \text{if we choose} \qquad \dot\phi = \nabla U \end{aligned}$$

which is the **time-reversed** down-hill path. Easy algorithms exist*.

*Weinan E, Weiqing Ren, and Eric Vanden-Eijnden. “String method for the study of rare events”. In: *Physical Review B* 66.5 (Aug. 2002), p. 052301. DOI: 10.1103/PhysRevB.66.052301.

Example: Pendulum

Consider **dampled pendulum**

$$\begin{cases} dx = v\,dt + \sigma\,dW_x, \\ dv = -\sin(x)\,dt - \gamma v\,dt + \sigma\,dW_v \end{cases}$$

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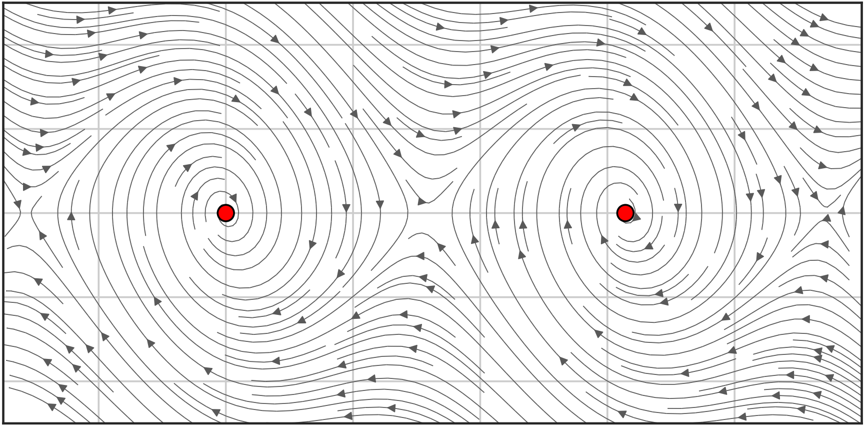

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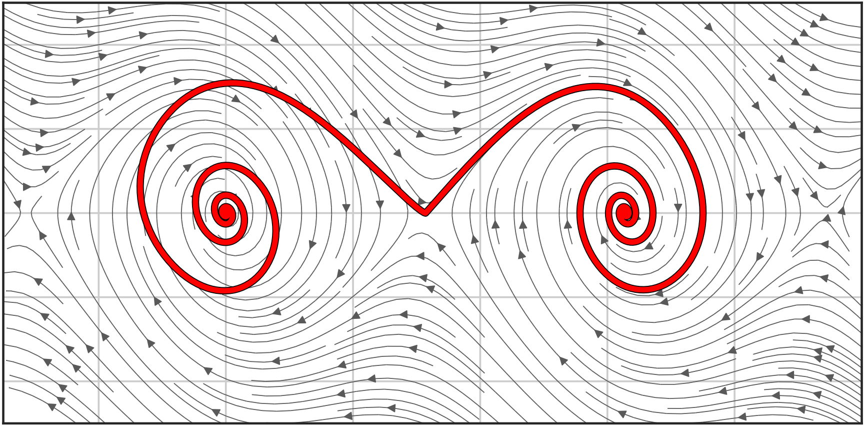

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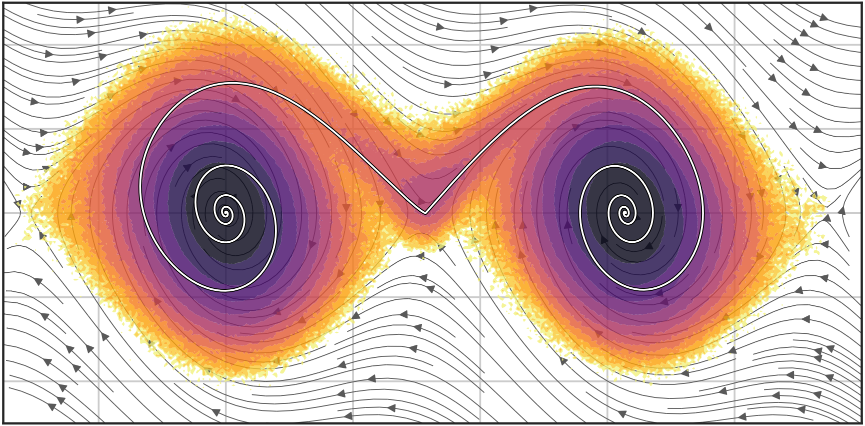

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or through **Hamiltionan**

$$H(x,p) = \sup_y \left\{ yp - L(x,y) \right\} \overset{\text{FW}}{=} b(x)p + \tfrac{1}{2} p \chi p$$

so that (ϕ^*, θ^*) fulfil **equations of motion**

$$\begin{cases} \dot{\phi} = \nabla_\theta H(\phi,\theta) & \overset{\text{FW}}{\Longrightarrow} \quad \dot{\phi} = b(\phi) + \chi\theta \\ \dot{\theta} = -\nabla_\phi H(\phi,\theta) & \overset{\text{FW}}{\Longrightarrow} \quad \dot{\theta} = -\nabla b(\phi)^T \theta \end{cases}$$

Finding the minimizer

Algorithm[†,‡]:

$$\dot{\phi} = b(\phi) + \chi\theta$$
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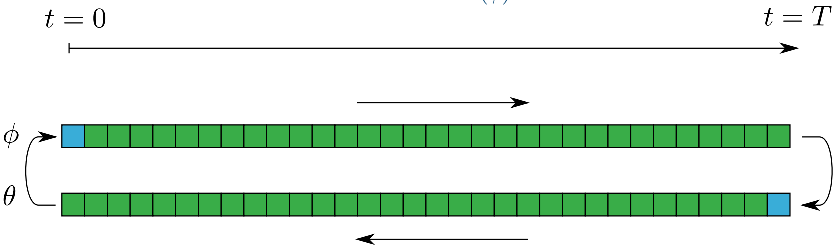

Advantages:

- Fits with the boundary conditions
- Simple time-integration scheme applicable (Runge-Kutta)
- No higher derivatives of $H(\phi, \theta)$
- This is essentially computing the gradient via the adjoint formalism

[†] A. I. Chernykh and M. G. Stepanov. "Large negative velocity gradients in Burgers turbulence". In: *Physical Review E* 64.2 (July 2001), p. 026306. DOI: 10.1103/PhysRevE.64.026306.

[‡] T. Grafke, R. Grauer, T. Schäfer, and E. Vanden-Eijnden. "Arclength Parametrized Hamilton's Equations for the Calculation of Instantons". In: *Multiscale Modeling & Simulation* 12.2 (Jan. 2014), pp. 566–580. ISSN: 1540-3459. DOI: 10.1137/130939158.

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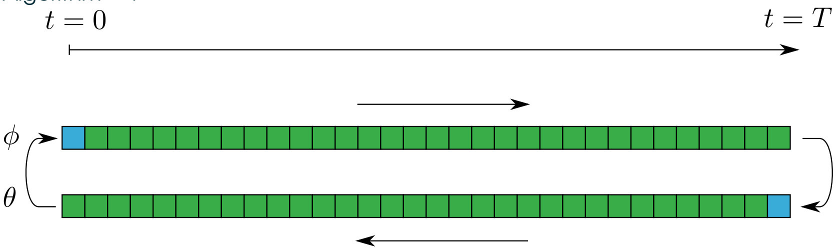

Problem for PDEs: **Memory**, e.g. 2D

$$\underbrace{2}_{(\phi,\theta)} \times \underbrace{1024 \times 1024}_{\text{space}} \times \underbrace{10^4}_{\text{time}} \approx 10^{10}$$

§ Antonio Celani, Massimo Cencini, and Alain Noullez. "Going forth and back in time: a fast and parsimonious algorithm for mixed initial/final-value problems". In: *Physica D: Nonlinear Phenomena* 195.3 (2004), pp. 283–291.

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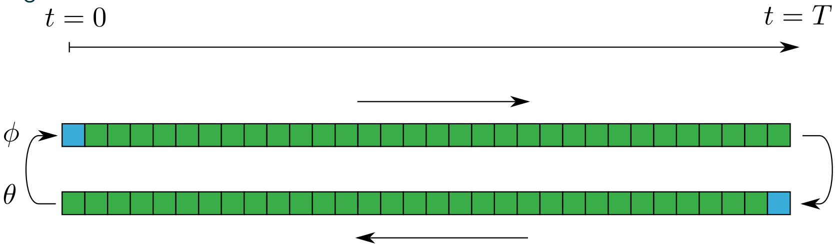

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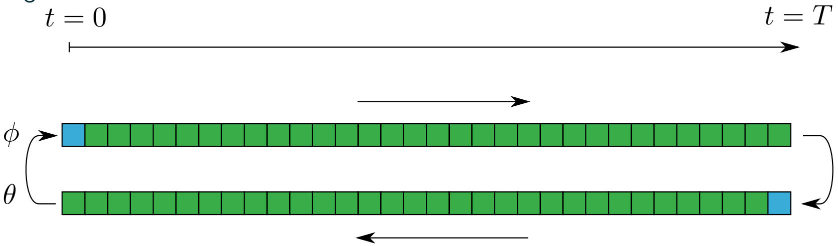

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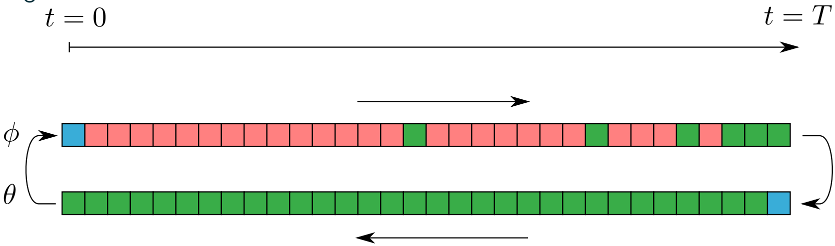

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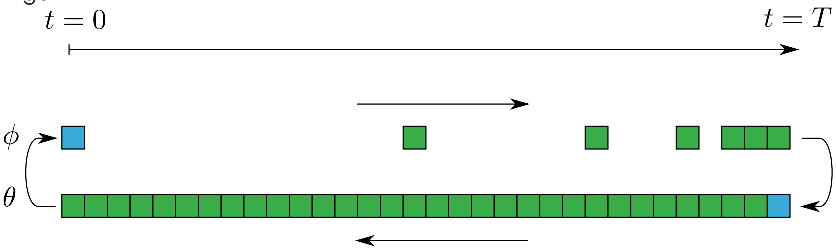

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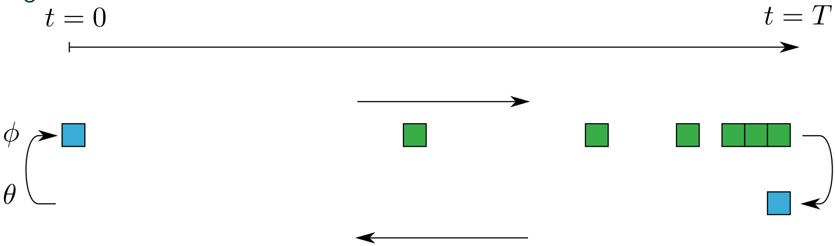

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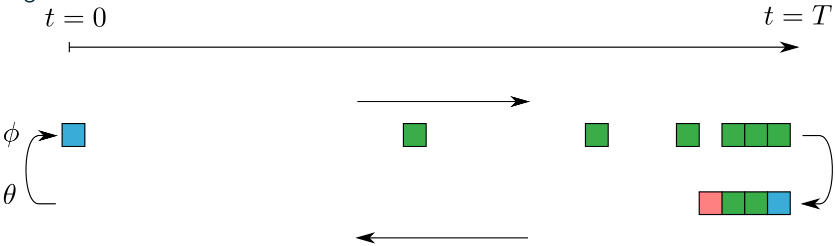

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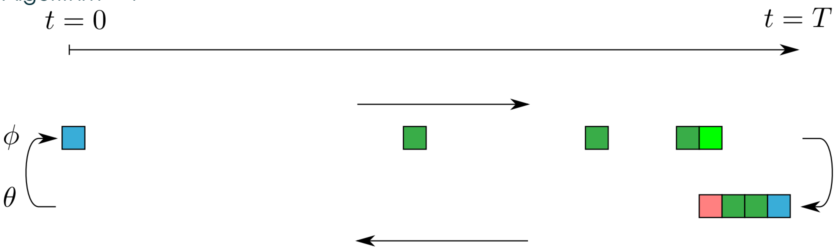

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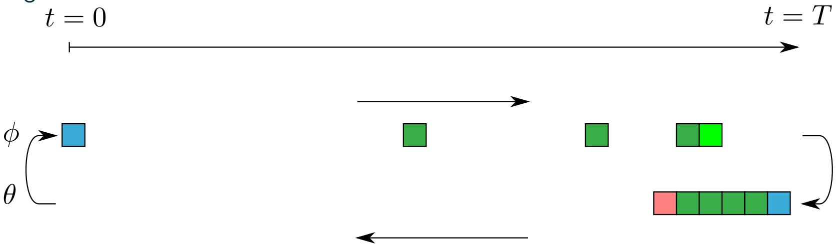

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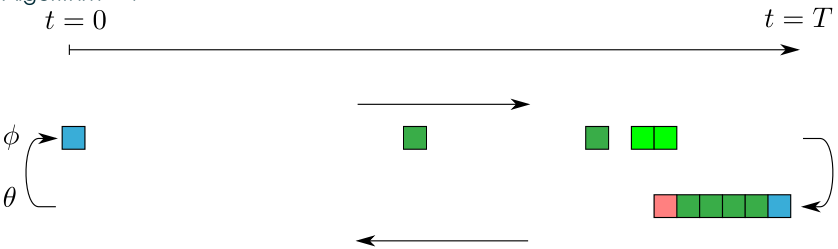

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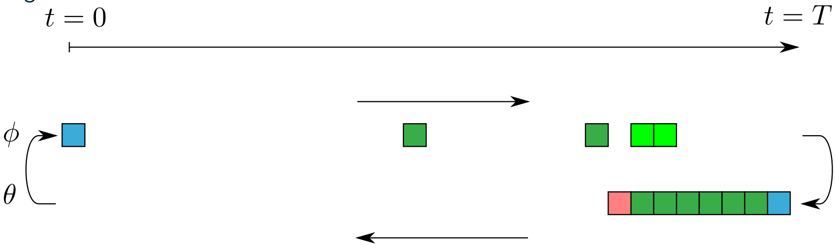

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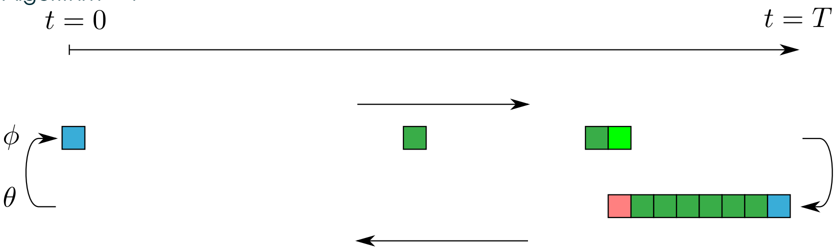

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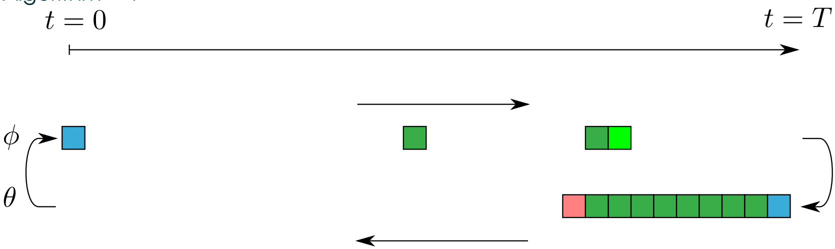

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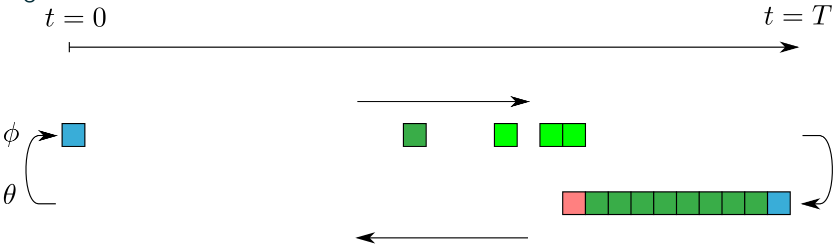

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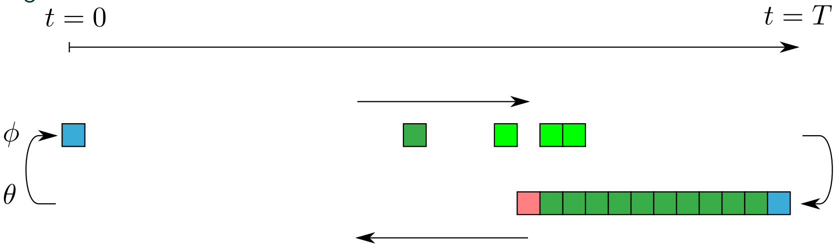

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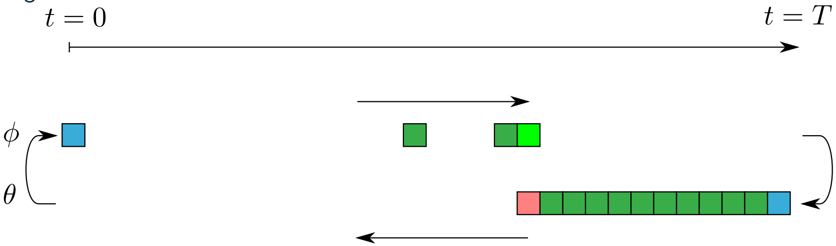

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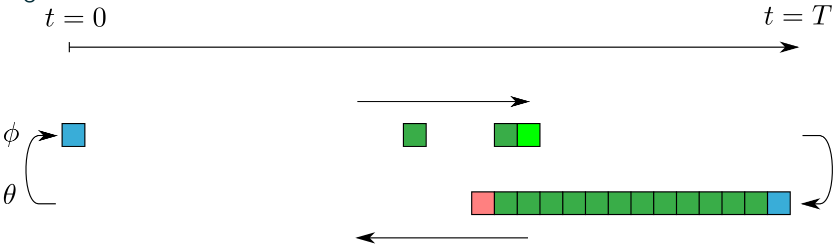

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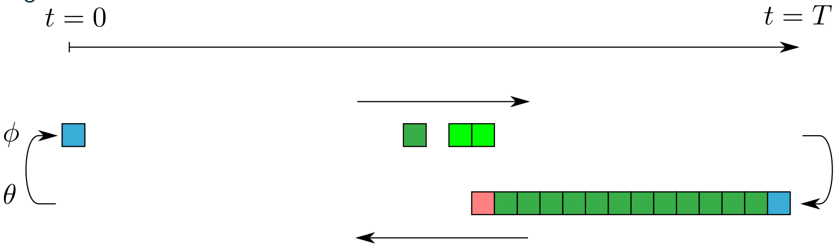

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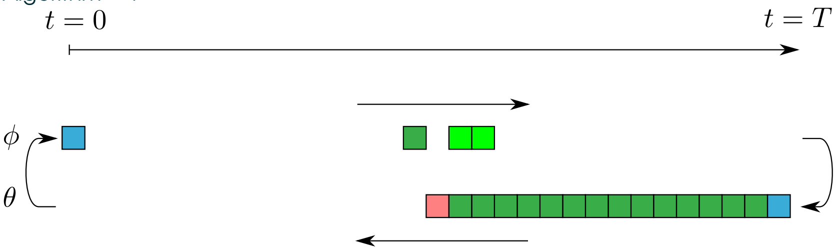

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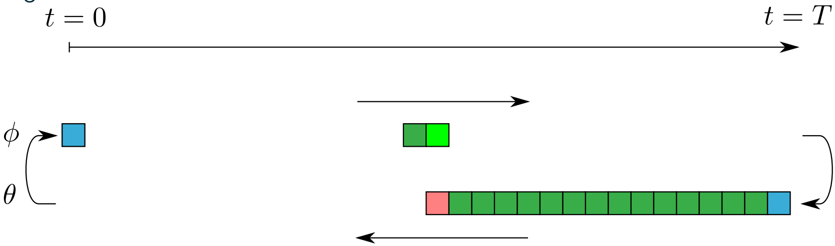

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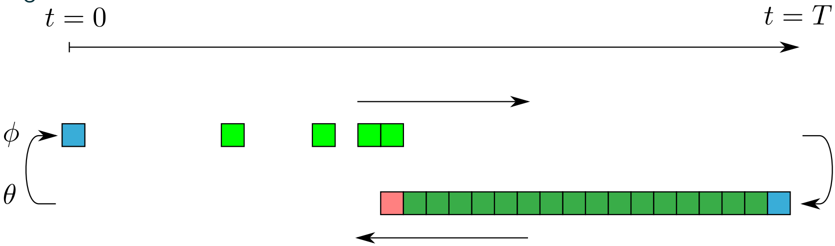

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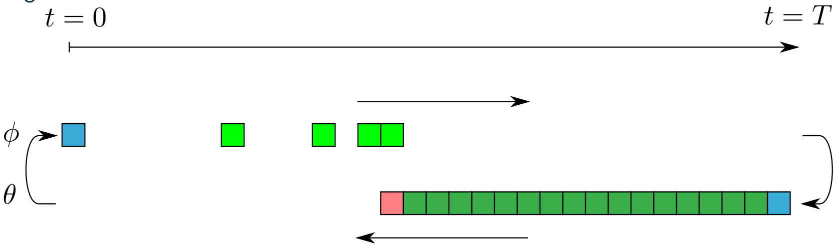

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- This is known as **"checkpointing"** in PDE optimization
- Additionally, bi-orthogonal wavelets to store fields

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Application: Extreme gradients in Burgers equation

Evolution of Burgers shocks:

$$u_t + uu_x - \nu u_{xx} = \eta$$

with

$$\langle \eta\eta' \rangle = \delta(t-t')\chi(x-x')$$

Compute

$$\mathcal{P}\left\{u_x(0,0) > z | u(x,-T) = 0\right\}$$

Question: What is the most likely evolution from $u(x)=0$ at $t=-\infty$, such that at the end (i.e. $t=0$) we have a high gradient in the origin $u_x(x=0,t=0)=z$ (shock)?

Grafke, Grauer, Schäfer, and Vanden-Eijnden 2015

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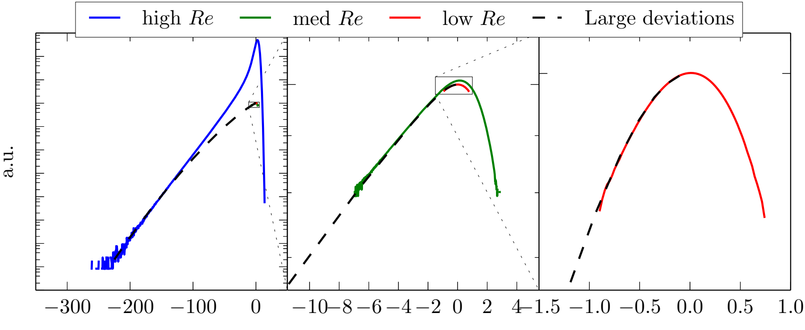

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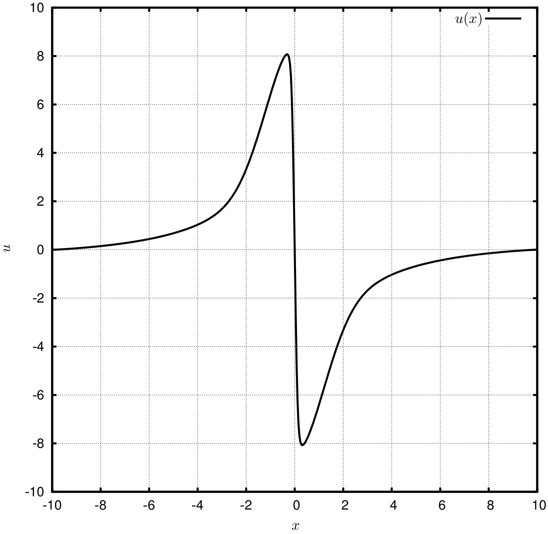
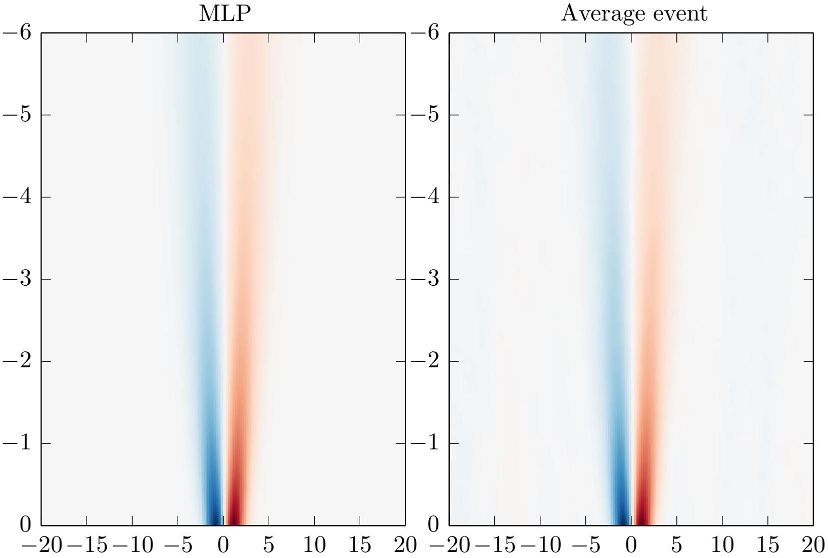


¶ Grafke, Grauer, and Schäfer 2013

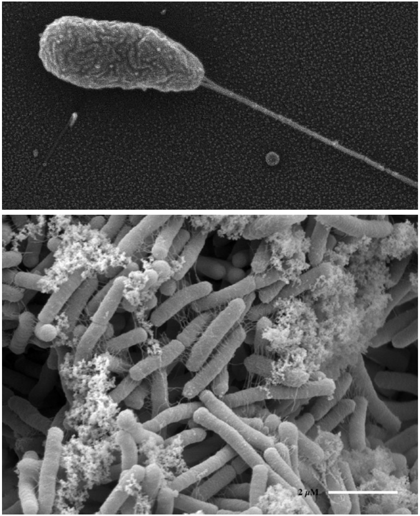
Application: Extreme gradients in Burgers turbulence

$$H(u,\theta) = \int \left(\theta \cdot (u \cdot \nabla u - \nu \nabla^2 u) + \tfrac{1}{2}\theta \chi \star \theta\right)\, dx$$



Bacteria show complex collective behavior

- have **active propulsion**, i.e. a free-swimming (planktonic) stage
- are able to sense their environment through **quorum sensing**
- stick to surfaces in **biofilms**



E. Coli: active propulsion & biofilms

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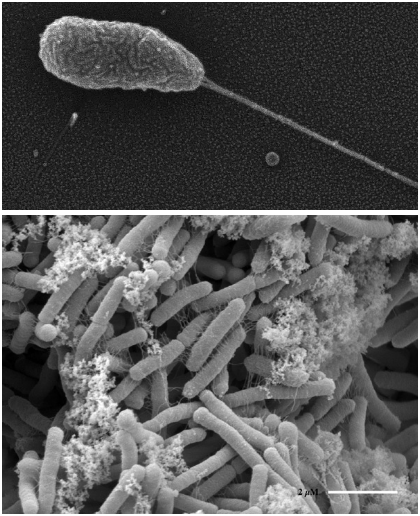
Model bacteria as N **agents** with

- **active** Brownian motion, i.e. velocity vector diffuses on a sphere,
- **density dependend** diffusion constant,
- and **birth/death**



E. Coli: active propulsion & biofilms

Application: Active matter phase separation

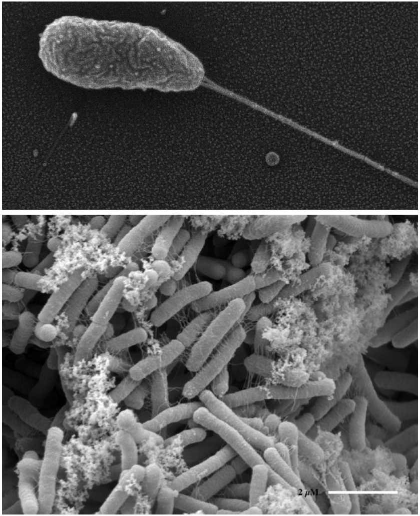
Bacteria show complex collective behavior

- have **active propulsion**, i.e. a free-swimming (planktonic) stage
- are able to sense their environment through **quorum sensing**
- stick to surfaces in **biofilms**

Model bacteria as N **agents** with

- **active** Brownian motion, i.e. velocity vector diffuses on a sphere,
- **density dependend** diffusion constant,
- and **birth/death**

Then take LDT for $N \to \infty$



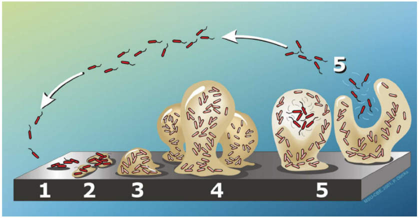
E. Coli: active propulsion & biofilms

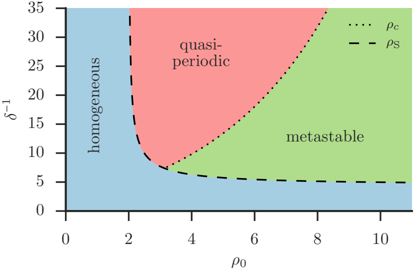
$$H(\rho,\theta) = \int \Big(\theta\partial_x(D_e(\rho)\partial_x\rho - \rho D(\rho)\partial_x(\delta^2\partial_x^2\rho + \theta)) + \alpha\rho(e^{\theta} - 1) + \alpha\rho^2/\rho_0(e^{-\theta} - 1)\Big)\, dx$$

Complex collective behaviour for simple active agents:

Propulsion and **Reproduction**

- When $\rho_0 < \rho_S$, **planktonic** phase is robust.
- When $\rho_S < \rho_0 < \rho_c$, particles oscillate between **biofilm** and **planktonic** phase
- When $\rho_c < \rho_0$, biofilms are **metastable**. They **rarely** disperse and reform by dying out
- Full **phase diagram** depends on carrying capacity ρ_0 and **domain size** δ^{-1}.





¶Tobias Grafke, Michael E. Cates, and Eric Vanden-Eijnden. "Spatiotemporal Self-Organization of Fluctuating Bacterial Colonies". In: *Physical Review Letters* 119.18 (Nov. 2017), p. 188003. DOI: 10.1103/PhysRevLett.119.188003

Application: Extreme ocean surface waves

Problem of **Rogue waves**:

- Creation mechanism not understood
- Probability unknown (but $>$ Gaussian)
- Measurements difficult
  (you might not be able to tell the tale)

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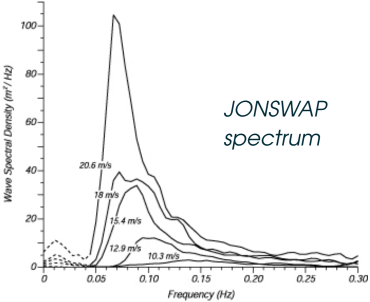

JONSWAP spectrum

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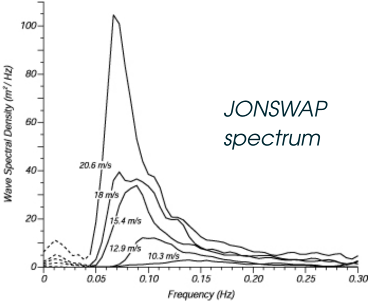

Strategy:

- **Random data** from **observation** as input
- Accurate **dynamical system** to extrapolate output (MNLS)

$$\partial_t u + \tfrac{1}{2}\partial_x u + \tfrac{i}{8}\partial_x^2 u - \tfrac{1}{16}\partial_x^3 u + \tfrac{i}{2}|u|^2 u + \tfrac{3}{2}|u|^2\partial_x u + \tfrac{1}{4}u^2\partial_x u^* - \tfrac{i}{2}|\partial_x||u|^2 = 0$$

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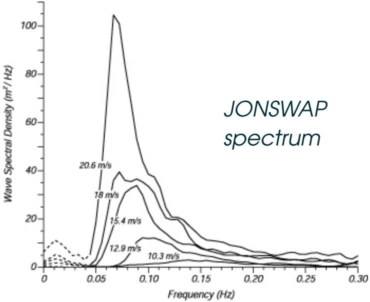
Strategy:

- **Random data** from **observation** as input
- Accurate **dynamical system** to extrapolate output (MNLS)
- Use LDT to obtain tails of height distribution



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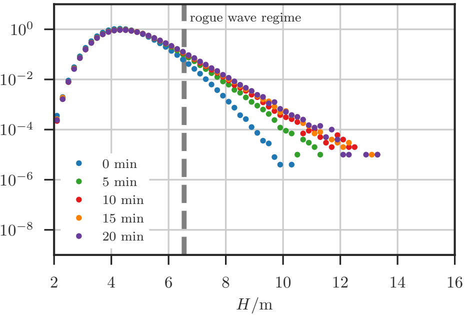
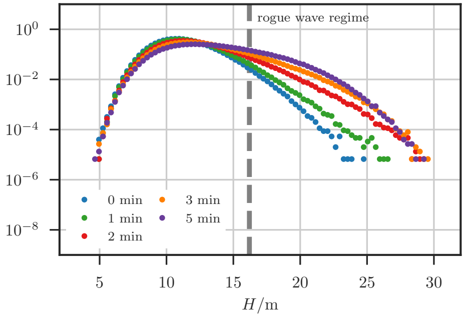
Application: Extreme ocean surface waves

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



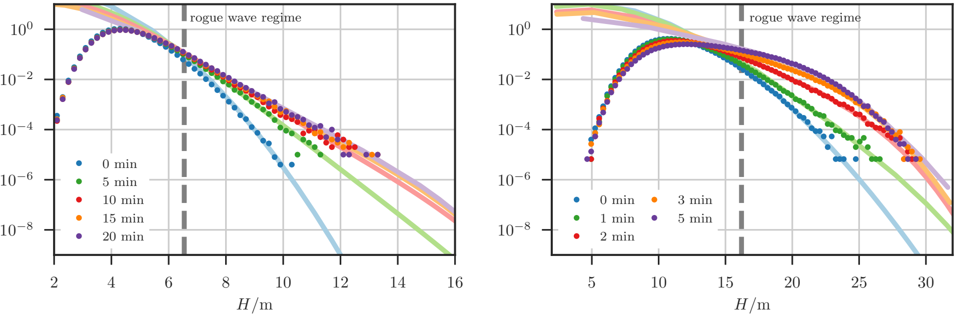
high sea ($H_s = 8.2$m, BFI $= 0.85$)



Probability disctribution of spatial maximum of surface height

Monte-Carlo simulation (dots)

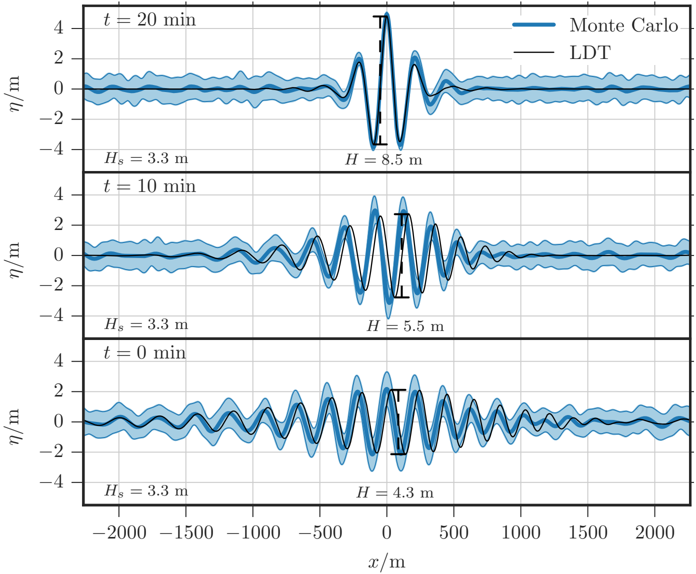
rough sea ($H_s = 3.3$m, BFI $= 0.34$)   *high* sea ($H_s = 8.2$m, BFI $= 0.85$)



Probability disctribution of spatial maximum of surface height

Comparison between **Monte-Carlo** simulation (dots) and **Large deviation theory** (lines)

Application: Extreme ocean surface waves



¶Giovanni Dematteis, Tobias Grafke, and Eric Vanden-Eijnden. "Rogue waves and large deviations in deep sea". In: *Proceedings of the National Academy of Sciences* 115.5 (Jan. 2018), pp. 855–860. ISSN: 0027-8424, 1091-6490. DOI: 10.1073/pnas.1710670115

LDT as WKB approximation

Consider Markov jump process with generator $\mathcal{L}$, s.t.

$$\partial_t f = \mathcal{L}^\dagger f \qquad \text{(forward Kolmogorov, Fokker-Planck, Master eqn)}$$

$$\partial_t f = \mathcal{L} f \qquad \text{(backward Kolmogorov)}$$

e.g. for diffusion above, $\mathcal{L} = b \cdot \nabla + \frac{1}{2}\varepsilon \nabla\nabla$

For **WKB** approximation, $f \sim \exp\left(\varepsilon^{-1} S\right)$, BKE becomes to leading order

$$\partial_t f = b \cdot \nabla S + \tfrac{1}{2}(\nabla S)^2$$

which is a **Hamilton-Jacobi** equation,

$$\partial_t f = H(x, \nabla S), \qquad H(x,p) = b \cdot p + \tfrac{1}{2} p^2$$

This is the **LDT Hamiltonian** from before(!), but works for all MJP

- for additive Gaussian SDE
- for Lévy processes
- other cases, i.e. stochastic averaging
- for multiplicative Gaussian SDE
- for jump process

We actually want the most probable event **regardless of duration**.

Drop the restriction of a pre-defined transition time T:

$$I(\tilde{\phi}) = \inf_{T\in(0,\infty)} \inf_{\phi} I_T(\phi)$$

Possibly attains minimum at $T \to \infty$.

Challenges: Infinite transition time and geometric rate function

We actually want the most probable event **regardless of duration**.

Drop the restriction of a pre-defined transition time T:

$$I(\tilde{\phi}) = \inf_{T\in(0,\infty)} \inf_{\phi} I_T(\phi)$$

Possibly attains minimum at $T \to \infty$. Since $H(\phi,\theta) = h = \text{cst}$, we have

$$\int L(\phi,\dot{\phi})\,dt = \int \sup_{\theta}\Big(\langle\dot{\phi},\theta\rangle - H(\phi,\theta)\Big)\,dt = \sup_{\theta:H(\phi,\theta)=h} \int \langle\dot{\phi},\theta\rangle\,dt + hT$$

Effectively:

Reduce minimisation over all paths to finding **geodesic** of the associated (almost Finsler) **metric**.

¶ Heymann, Vanden-Eijnden (2008), Grafke, Schäfer, Vanden-Eijnden (2017)

Main theme

Obtain **statistics** of and **structures** for rare events by numerically computing **large deviation minimisers** for spatially extended systems

Challenges:

- Analytic solutions not available
- Needs **PDE constrained optimisation** (on GPUs)
- Simplification necessary through nature of problem

Applications:

- Fluid dynamic
- Non-equilibrium stat. mech.
- Rogue waves