# Population dynamics and rare events

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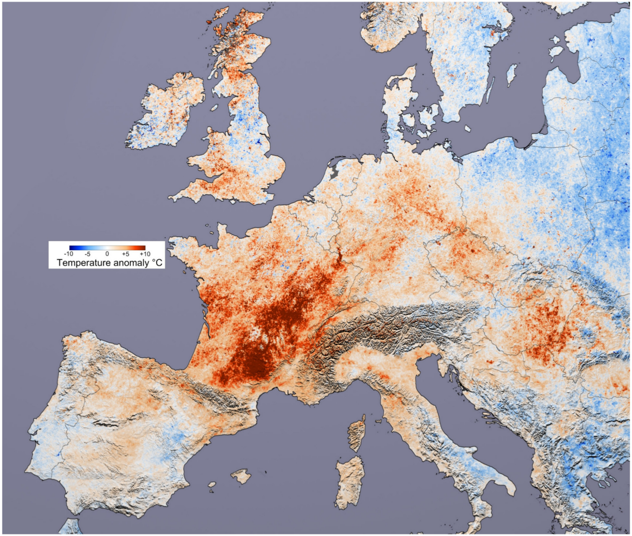
PSM Group Meeting — 27 March 2017

# Why studying rare events?




2003 heat wave, Europe [Terra MODIS]

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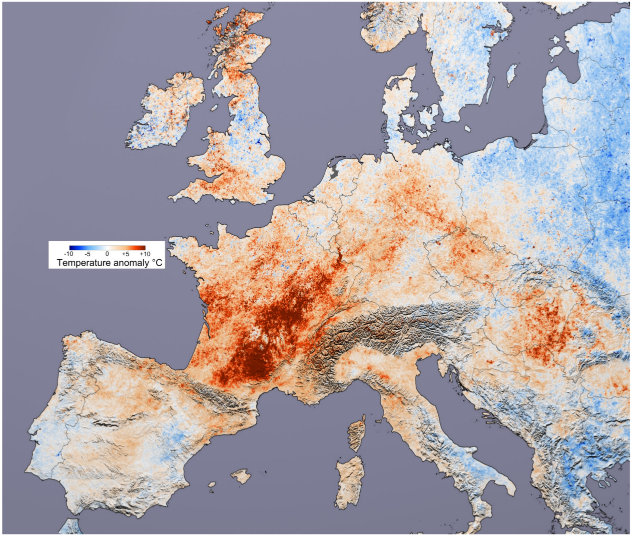


[Anomaly for **1-month** average] 2003 heat wave, Europe [Terra MODIS]

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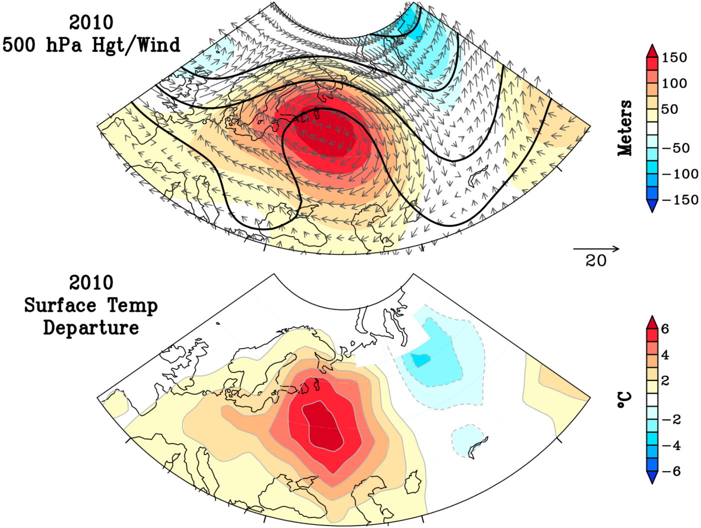


2010 heat wave in Western Russia [Dole *et al.*, 2011]

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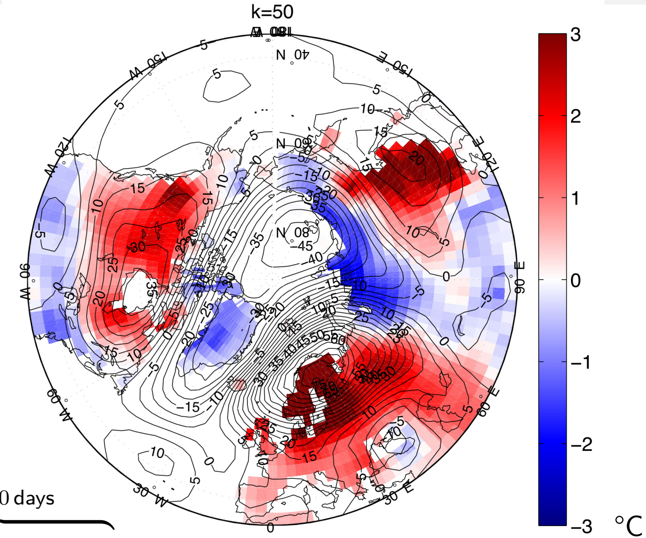


$$\overbrace{\frac{1}{t_{\max}}\int_0^{t_{\max}}}^{t_{\max}=40\text{ days}} dt\, \Delta T(t) > 2^\circ C \Rightarrow$$ « Teleconnection patterns » [Bouchet *et al.*]

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Questions for physicists:

- Probability and **dynamics** of rare events?
- How to sample these in numerical modelisations?
- Numerical **tools and methods** to understand their formation?

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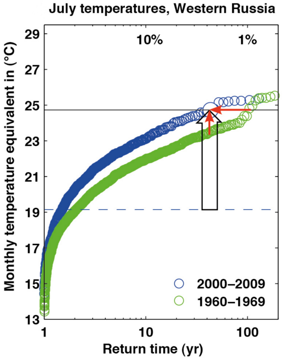


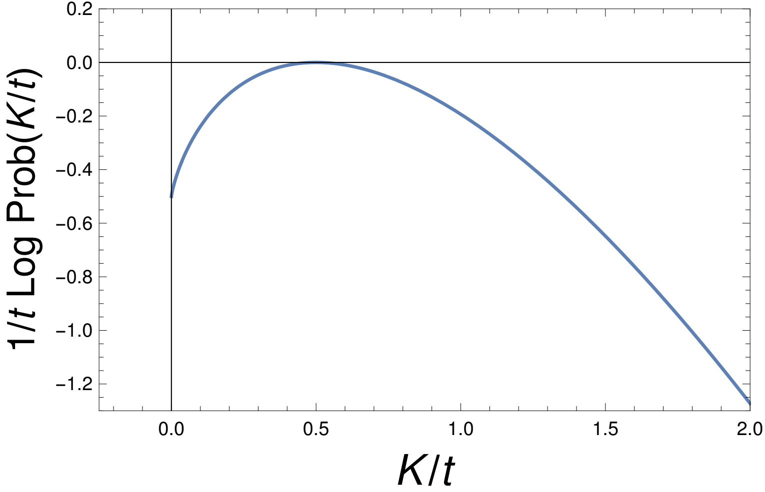

Evolution of the return time
of the monthly averaged temperature

$$\frac{1}{t_{\max}} \int_0^{t_{\max}} dt\ T(t)$$

Due anthropogenic impact on climate?

[Otto *et al.*, 2012]

# Distribution of a time-extensive observable $K$

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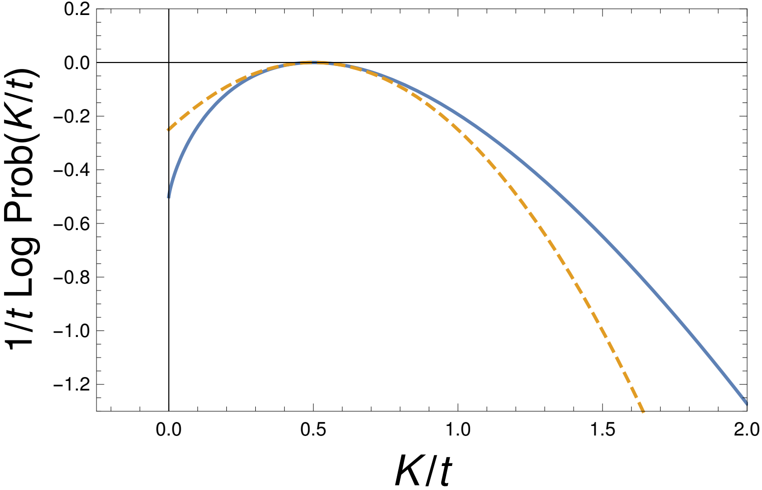


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# $s$-modified dynamics

- Markov processes:

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big\{ \underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},t)}_{\text{loss term}} \Big\}$$

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## $s$-modified dynamics $\qquad K = k_{\mathcal{C}_0\mathcal{C}_1} + k_{\mathcal{C}_1\mathcal{C}_2} + \dots$

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# Numerical method [with J. Tailleur]

## Evaluation of large deviation functions [*à la* Monte-Carlo diffusion]

$$\sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t) = \left\langle \mathrm{e}^{-s\,K} \right\rangle \sim \mathrm{e}^{t\,\psi(s)}$$

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
- continuous time: Lecomte, Tailleur [JSTAT P03004 (2007)]

## Cloning dynamics

$$\partial_t \hat{P}(\mathcal{C}, s) = \underbrace{\sum_{\mathcal{C}'} W_s(\mathcal{C}' \to \mathcal{C})\hat{P}(\mathcal{C}', s) - r_s(\mathcal{C})\hat{P}(\mathcal{C}, s)}_{\text{modified dynamics}} \; + \underbrace{\delta r_s(\mathcal{C})\hat{P}(\mathcal{C}, s)}_{\text{cloning term}}$$

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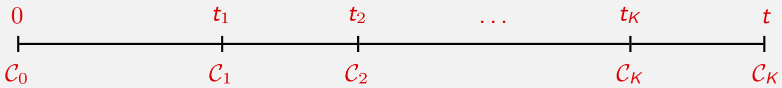
# Explicit construction (1/3)




## Probability-preserving contribution

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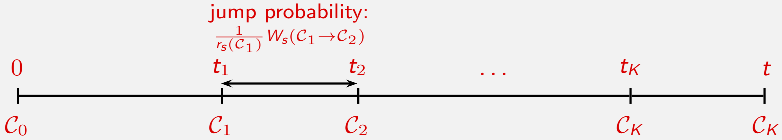



## Which configurations will be visited?

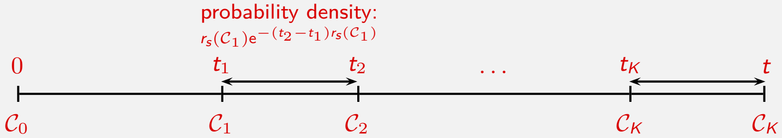
Configurational part of the trajectory: $\mathcal{C}_0 \to \dots \to \mathcal{C}_K$

$$\text{Prob}\{\text{hist}\} = \prod_{n=0}^{K-1} \frac{W_s(\mathcal{C}_n \to \mathcal{C}_{n+1})}{r_s(\mathcal{C}_n)}$$

where

$$r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}')$$

# Explicit construction (2/3)




## When shall the system jump from one configuration to the next one?

- probability density for the time interval $t_n - t_{n-1}$

$$r_s(\mathcal{C}_{n-1})\mathrm{e}^{-(t_n-t_{n-1})r_s(\mathcal{C}_{n-1})}$$

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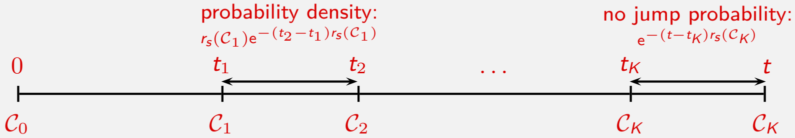


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- probability not to leave $\mathcal{C}_K$ during the time interval $t - t_K$

$$e^{-(t-t_K)r_s(\mathcal{C}_K)}$$

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**How to take into account loss/gain of probability?**

- handle a large number of copies of the system
- implement a selection rule: on a time interval $\Delta t$ a copy in config $\mathcal{C}$ is replaced by $e^{\Delta t\,\delta r_s(\mathcal{C})}$ copies
- $\psi(s)$ = the rate of exponential growth/decay of the total population
- optionally: keep population constant by non-biased pruning/cloning

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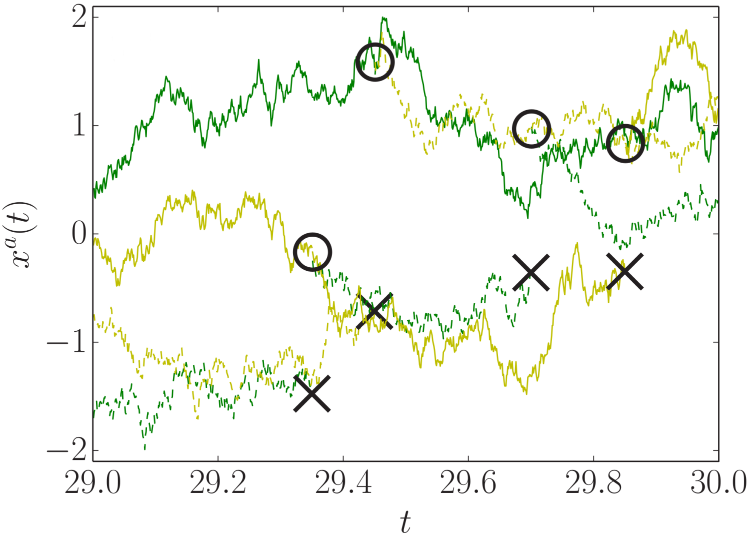
## Biological interpretation

- copy in configuration $\mathcal{C} \equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates $W_s \equiv$ **mutations**
- cloning at rates $\delta r_s \equiv$ **selection** rendering atypical histories typical

# An example: $4$ copies, $1$ degree of freedom $\mathcal{C} = x \in \mathbb{R}$



# How to perform averages? (i) [with R Jack, F Bouchet, T Nemoto]

⋆ Final-time distribution: *proportion* of copies in $\mathcal{C}$ at $t$

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Final-time distribution governed by **right** eigenvector.

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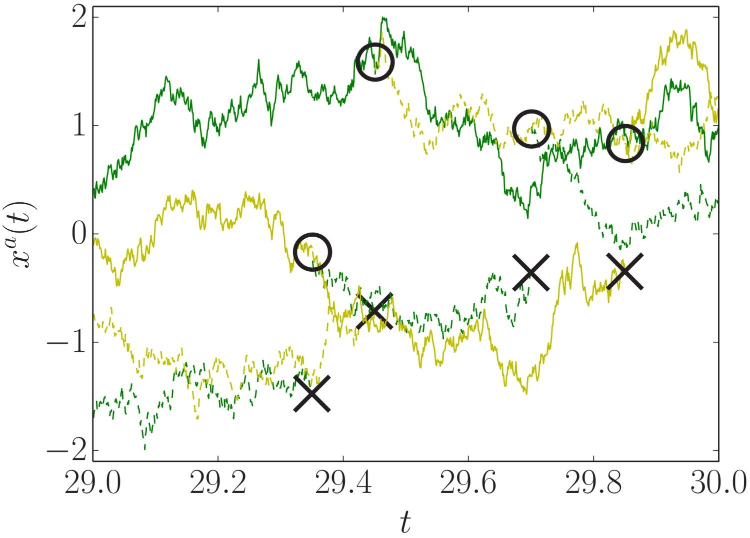

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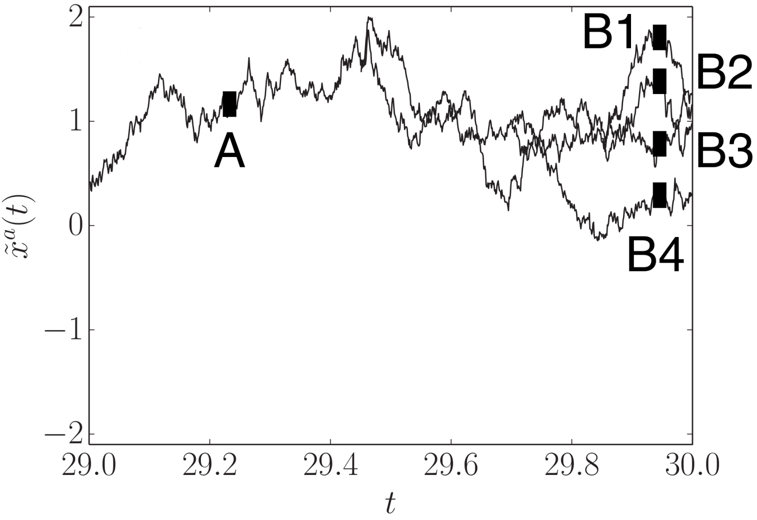
$$p(t|\mathcal{C},t_1) = \frac{\langle N_{\rm nc}(t|\mathcal{C},t_1)\rangle_s}{\langle N_{\rm nc}(t)\rangle_s} \underset{t\to\infty}{\sim} \langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle \equiv p_{\rm ave}(\mathcal{C})$$

Mid-time distribution governed by **left** and **right** eigenvectors.

# An example: $4$ copies, $1$ degree of freedom $\mathcal{C} = x \in \mathbb{R}$




Huge sampling issue

# How to perform averages?

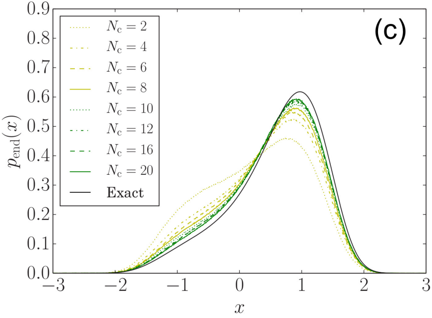
- ⋆ Mid-time ancestor distribution:

  fraction of copies (at time $t_1$) which were in configuration $\mathcal{C}$, knowing that there are in configuration $\mathcal{C}_\mathsf{f}$ at final time $t_\mathsf{f}$:

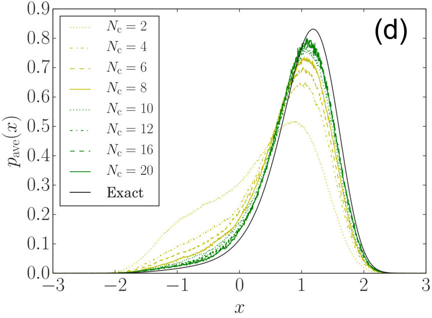
$$p_{\mathsf{anc}}(\mathcal{C}, t_1; \mathcal{C}_\mathsf{f}, t_\mathsf{f}) = \frac{\langle N_{\mathsf{nc}}(\mathcal{C}_\mathsf{f}, t_\mathsf{f}|\mathcal{C}, t_1)\rangle_s}{\sum_{\mathcal{C}'}\langle N_{\mathsf{nc}}(\mathcal{C}_\mathsf{f}, t_\mathsf{f}|\mathcal{C}', t_1)\rangle_s} \underset{t_{\mathsf{f},1}\to\infty}{\sim} \langle L|\mathcal{C}\rangle\langle\mathcal{C}|R\rangle = p_{\mathsf{ave}}(\mathcal{C})$$

**The "ancestor statistics" of a configuration $\mathcal{C}_\mathsf{f}$ is thus independent (far enough in the past) of the configuration $\mathcal{C}_\mathsf{f}$.**

# Example distributions for a simple Langevin dynamics

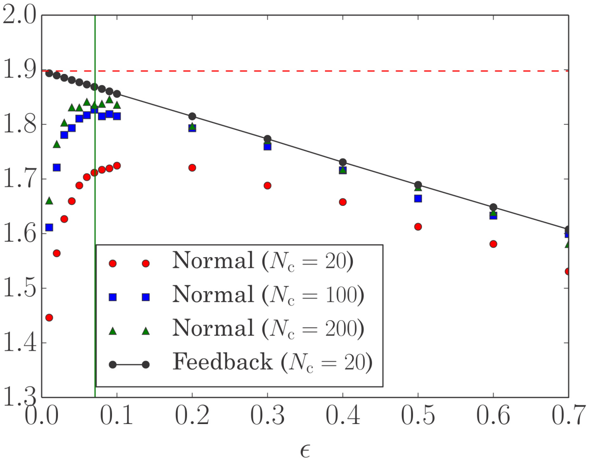



final-time: $p_{\mathsf{end}}(x)$




intermediate-time: $p_{\mathsf{ave}}(x)$

# The small-noise crisis: systematic errors grow as $\epsilon \to 0$




Cause: as $\epsilon \to 0$, $p_{\text{ave}}(x)$ & $p_{\text{end}}(x)$ → sharply peaked at *different points*
*i.e.* the clones do not ~~attack~~ sample correctly the phase space

# How to make mid- and final-time distribution closer?

Driven/auxiliary dynamics: [Maes, Jack&Sollich, Touchette&Chetrite]

- Probability preserving
- No mismatch between $p_{\text{ave}}$ and $p_{\text{end}}$
- Constructed as

$$\mathbb{W}_s^{\text{aux}} = L\mathbb{W}_s L^{-1} - \psi(s)\mathbf{1}$$

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- Issue: determining $L$ is difficult
- Solution: evaluate $L$ as $L_{\mathrm{test}}$ on the fly and simulate

$$\mathbb{W}_s^{\mathrm{test}} = L_{\mathrm{test}} \mathbb{W}_s L_{\mathrm{test}}^{-1}$$

- Whichever $L_{\mathrm{test}}$, the simulation is still correct. **Iterate**

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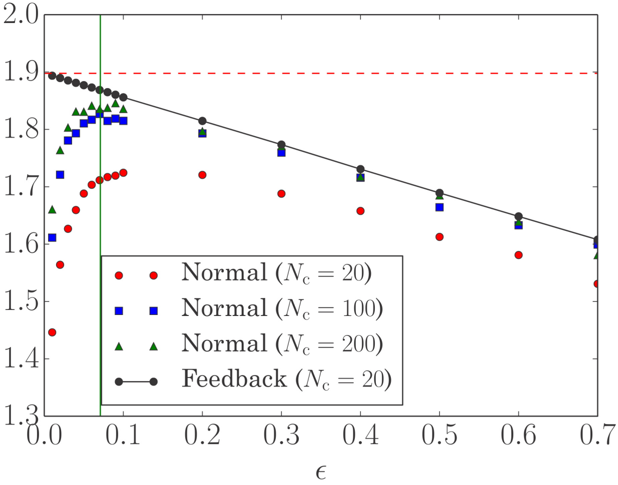
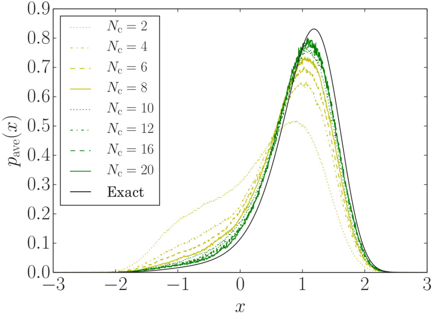
Similar in spirit to **multi-canonical** (e.g. Wang-Landau) approach in static thermodynamics

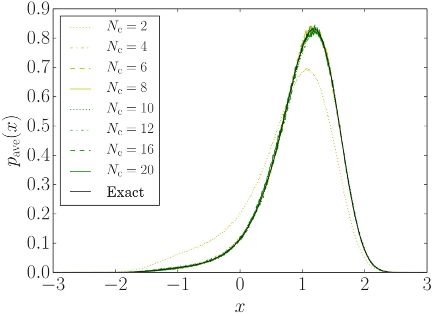
# Improvement of the small-noise crisis (i.i)




Physical insight: probability loss transformed into *effective forces*

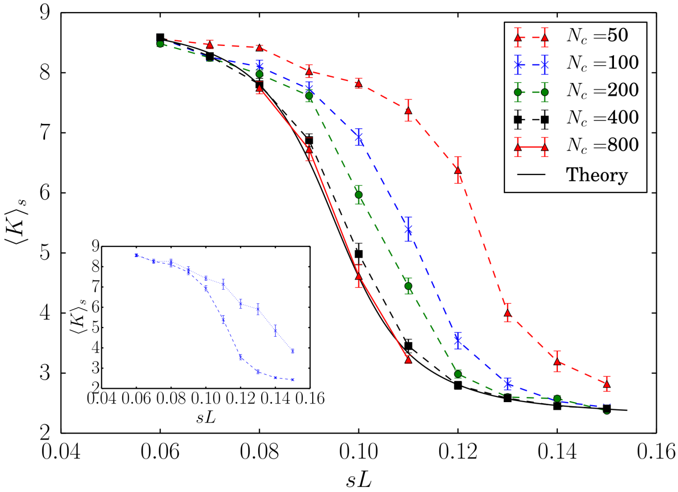
# Improvement of the small-noise crisis (i.ii)




Much more efficient evaluation of the biased distribution.
Even for a very crude (polynomial) approximation of the effective force.

# Improvement of the small-noise crisis (ii)




Interacting system in 1D.

Effective force: 1-, 2-, 3- body interactions only [also crude approx.].

# Summary and questions (1)

**Multicanonical approach** [with F Bouchet, R Jack, T Nemoto]

- Sampling problem (depletion of ancestors)
- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom

# Summary and questions (1)

## Multicanonical approach [with F Bouchet, R Jack, T Nemoto]

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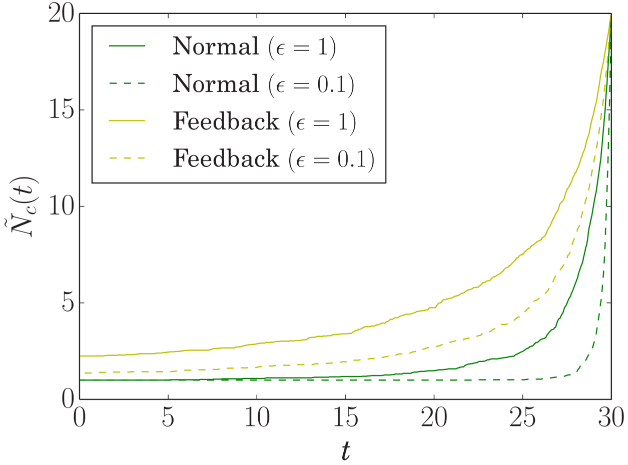
## Finite-population effects [with E Guevara, T Nemoto]

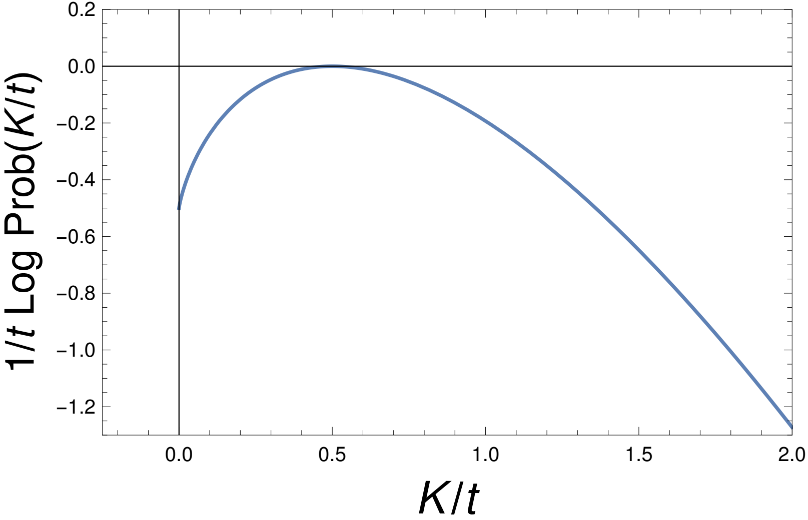
- Quantitative finite-$N_{\mathrm{clones}}$ scaling $\rightarrow$ interpolation method
- Initial transient regime due to small population
- Analogy with biology: many small islands *vs.* few large islands?
- Question: effective forces $\leftarrow$ selection?

# Questions (2): why is it working?

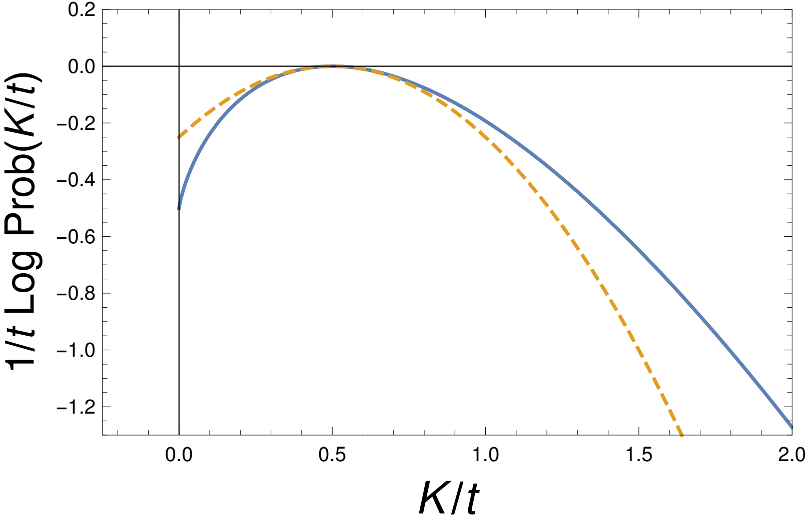
Improvement of the depletion-of-ancestors problem:




Dashed line: lower noise    Continuous line: higher noise




$$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$$

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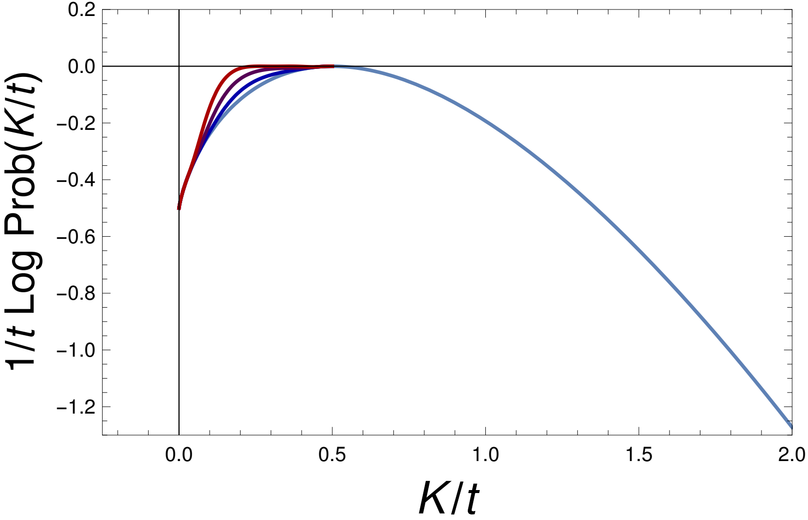


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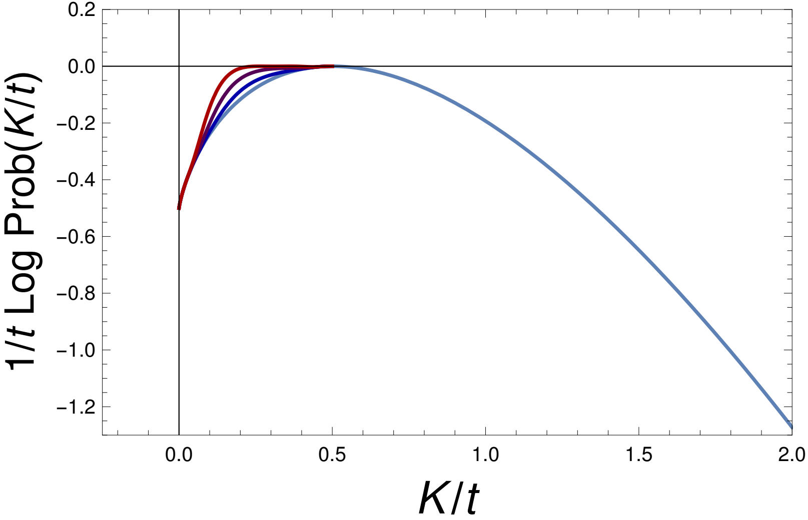
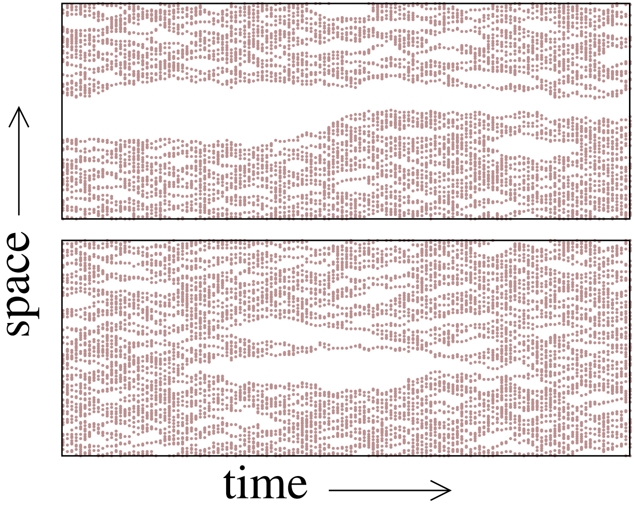
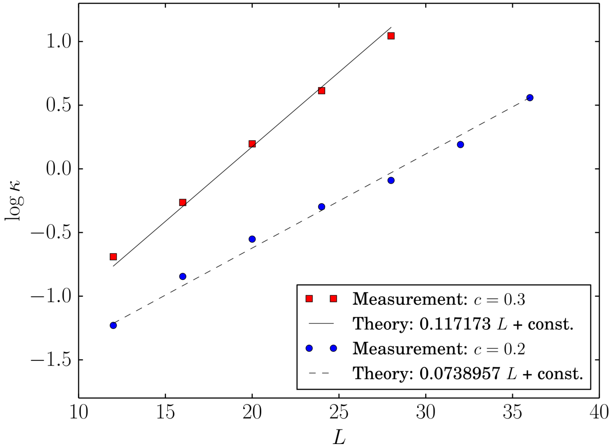



$\mathrm{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.




[Merrolle, Garrahan and Chandler, 2005]




Exponential divergence of the susceptibility