Population dynamics method for rare events: systematic errors & feedback control

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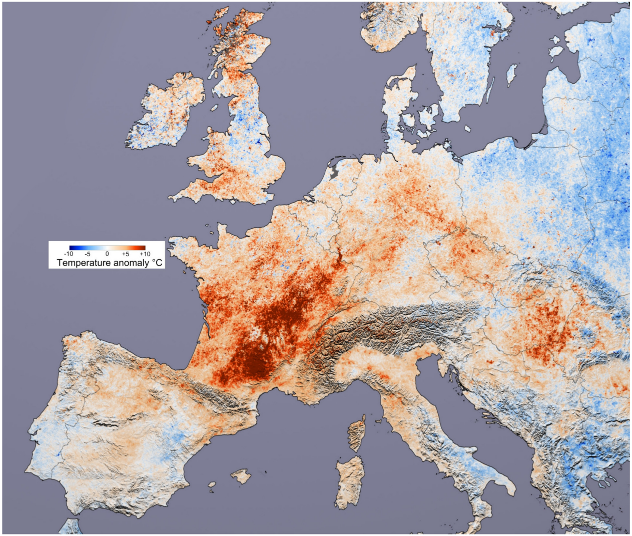
Why studying rare events?



2003 heat wave, Europe [Terra MODIS]

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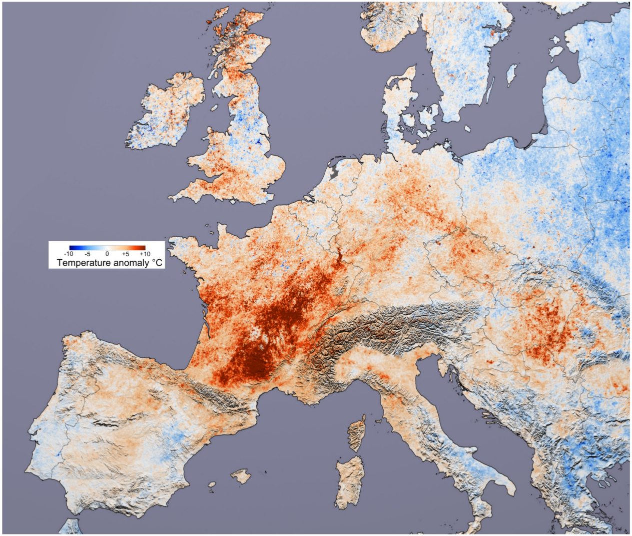

[Anomaly for **1-month** average] 2003 heat wave, Europe [Terra MODIS]

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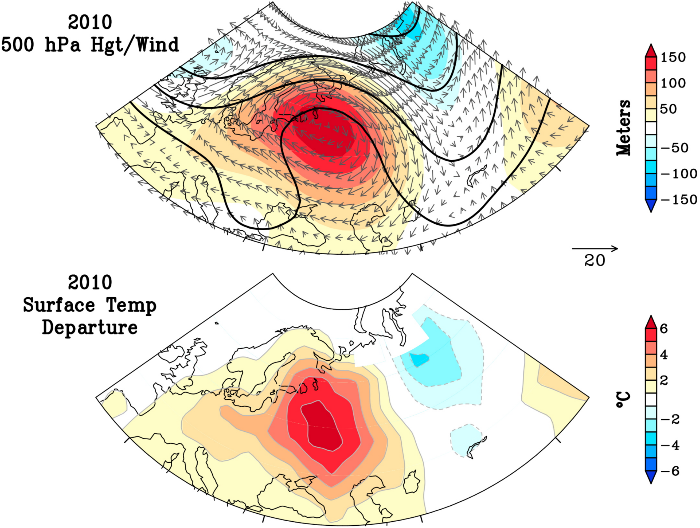

2010 heat wave in Western Russia [Dole *et al.*, 2011]

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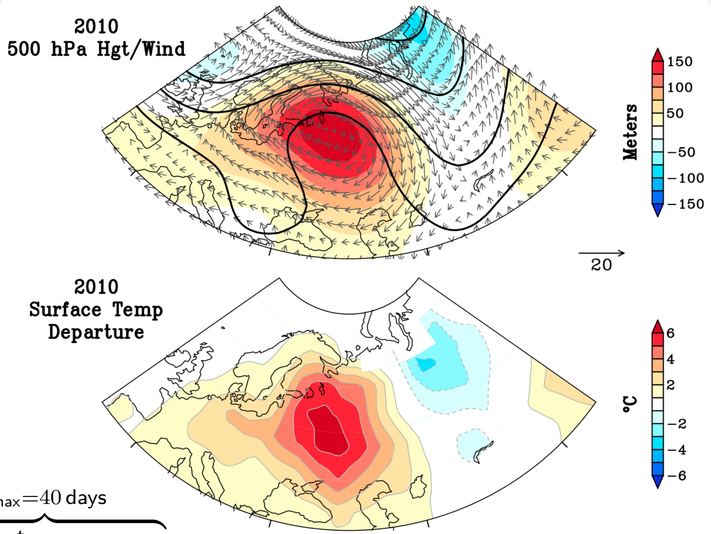

°C

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

Why studying rare events?

Questions for physicists and mathematicians:

- 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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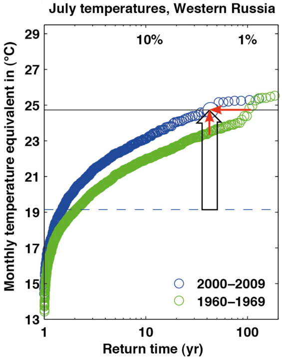


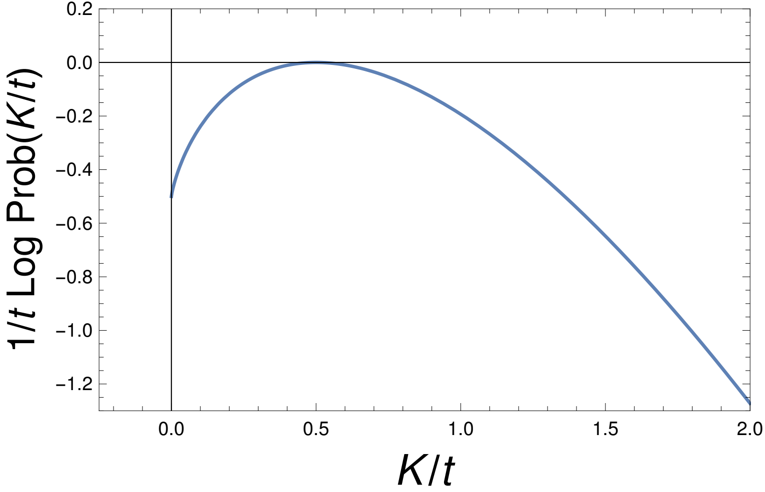
Evolution of the return time
of the monthly averaged temperature

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

Due anthropogenic impact on climate?

[Otto *et al.*, 2012]

Distribution of a time-extensive observable K



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

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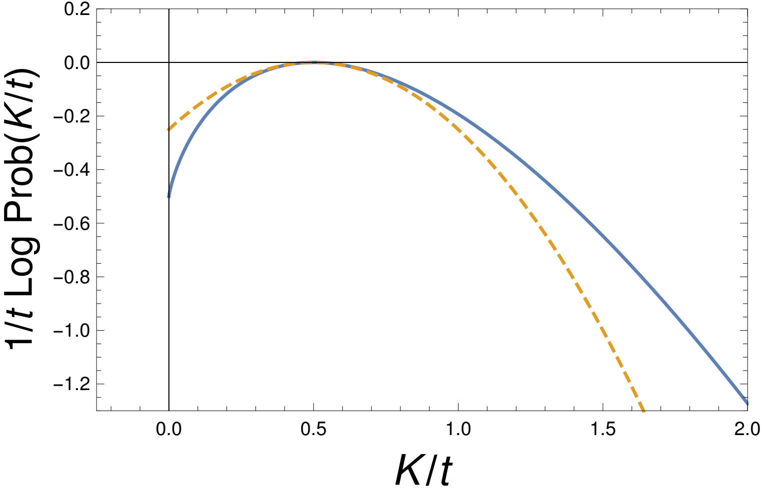

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s-modified dynamics

- 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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Numerical method [JB Anderson; D Aldous; P Grassberger; P Del Moral; ...]

Evaluation of large deviation functions [*à la* "Diffusion Monte-Carlo"]

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

- discrete time: Giardinà, Kurchan, Peliti [PRL **96**, 120603 (2006)]
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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 Δt 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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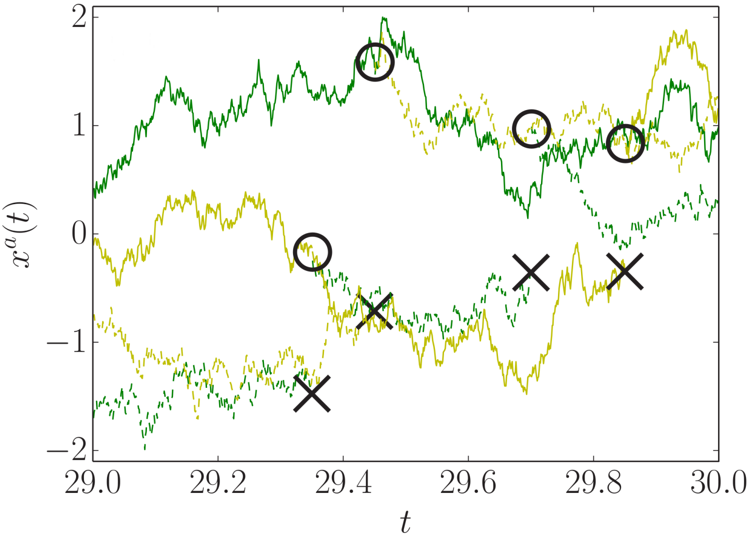
Biological interpretation

- copy in configuration $\mathcal{C}$ $\equiv$ organism of **genome** $\mathcal{C}$
- dynamics of rates W_s $\equiv$ **mutations**
- cloning at rates δr_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

$$\langle N_{\rm nc}(t)\rangle_s$$

$$\langle N_{\rm nc}(\mathcal{C},t)\rangle_s$$

$$p_{\rm end}(\mathcal{C},t) = \frac{\langle N_{\rm nc}(\mathcal{C},t)\rangle_s}{\langle N_{\rm nc}(t)\rangle_s}$$

[$N_{\rm nc}$ = number in non-constant population dynamics]

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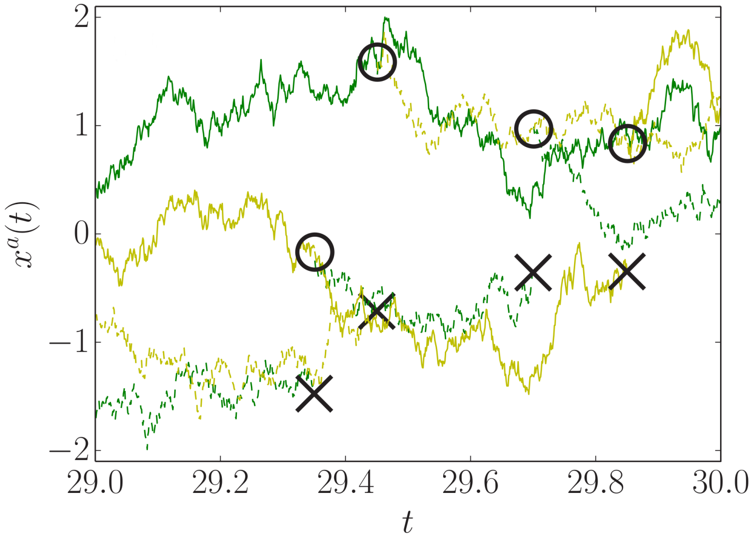
[$N_{\rm nc}$ = number in non-constant population dynamics]

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

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



How to perform averages? (ii) Intermediate times

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

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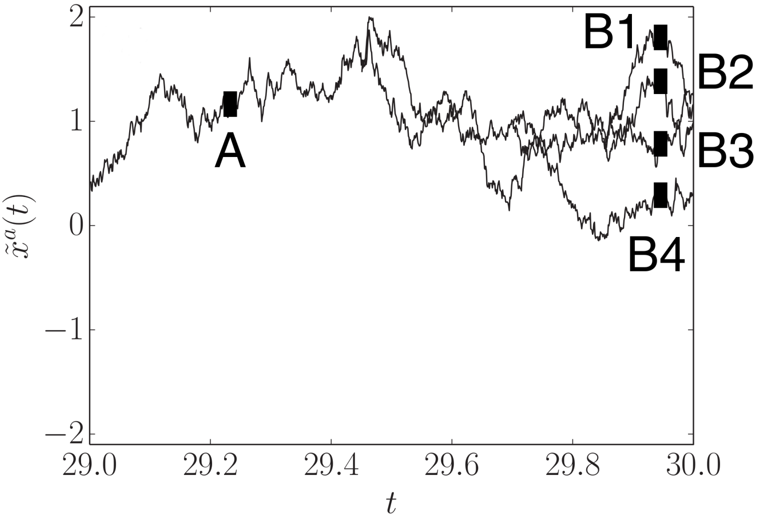


Huge sampling issue

How to perform averages?

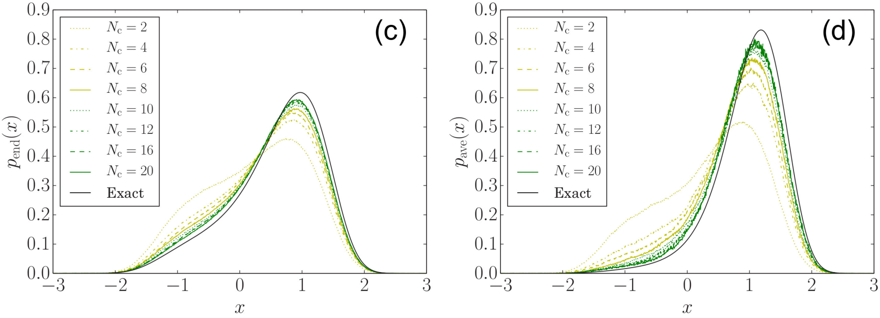
- ⋆ Mid-time ancestor distribution:

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

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

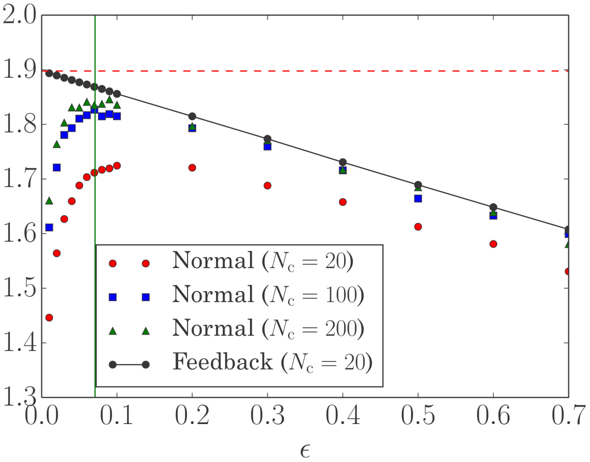
The “ancestor statistics” of a configuration $\mathcal{C}_\mathrm{f}$ is thus independent (far enough in the past) of the configuration $\mathcal{C}_\mathrm{f}$.

Example distributions for a simple Langevin dynamics



final-time: $p_{\text{end}}(x)$ intermediate-time: $p_{\text{ave}}(x)$

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



Cause: as $\epsilon \to 0$, $p_{\text{ave}}(x)$ & $p_{\text{end}}(x) \to$ 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]

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- No mismatch between p_{ave} and p_{end}
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- No mismatch between p_{ave} and p_{end}
- Constructed as

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

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

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

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

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

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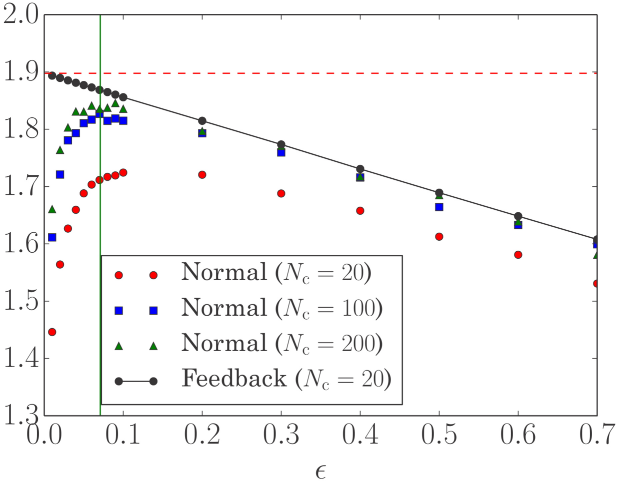
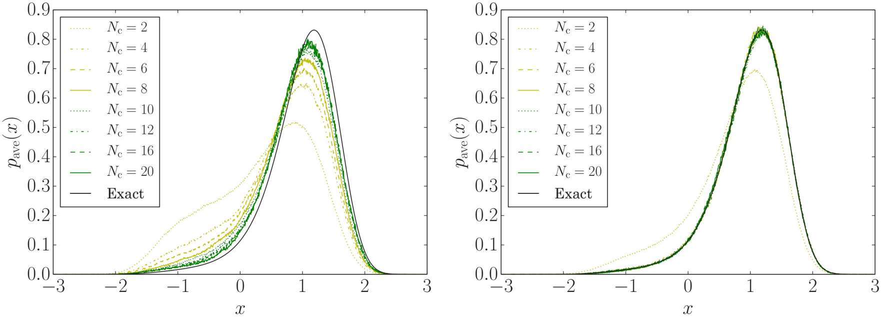
Similar in spirit to **multi-canonical** (e.g. Wang-Landau) approach in static thermodynamics

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



Physical insight: probability loss transformed into *effective forces*

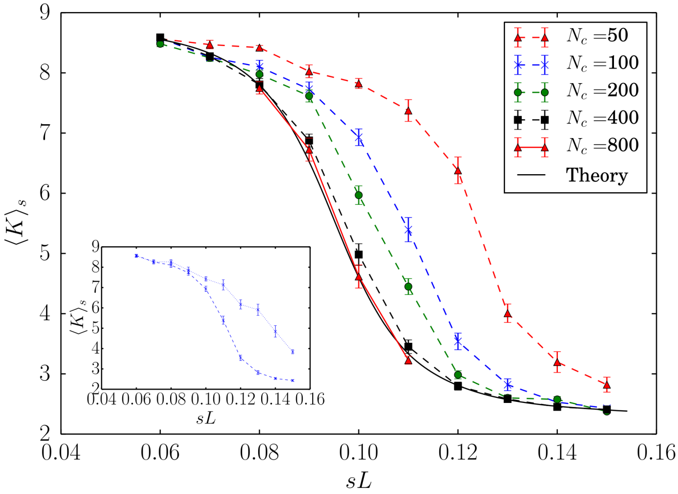
Improvement of the small-noise crisis (i.ii)



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

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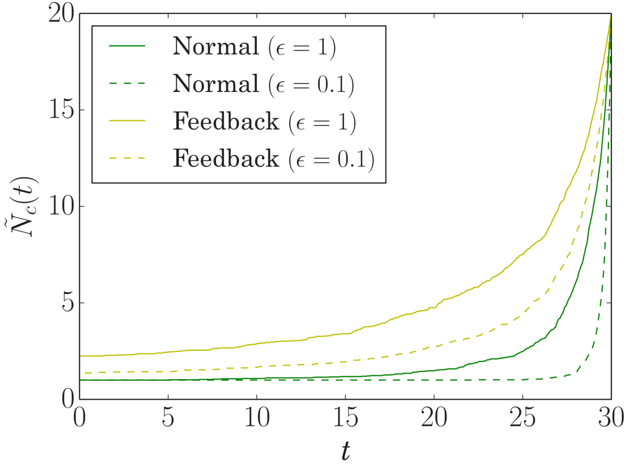
- Systems with large number of degrees of freedom

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

- Quantitative finite-N_{clones} scaling $\to$ 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?

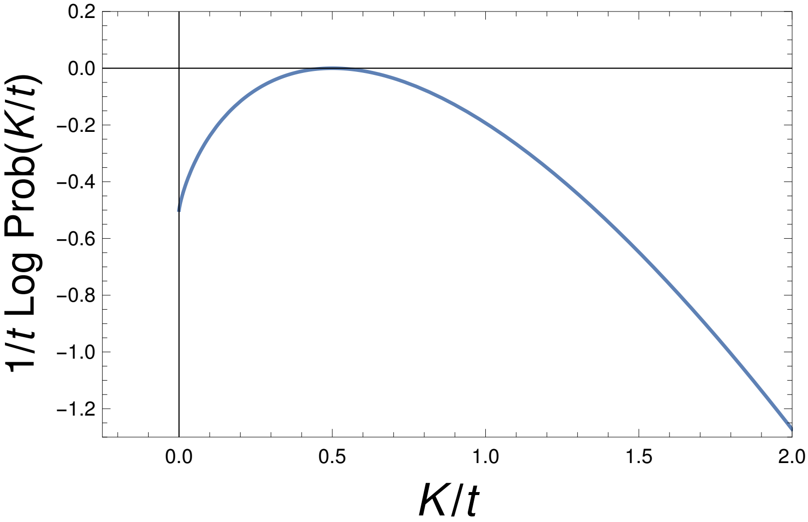
Improvement of the depletion-of-ancestors problem:



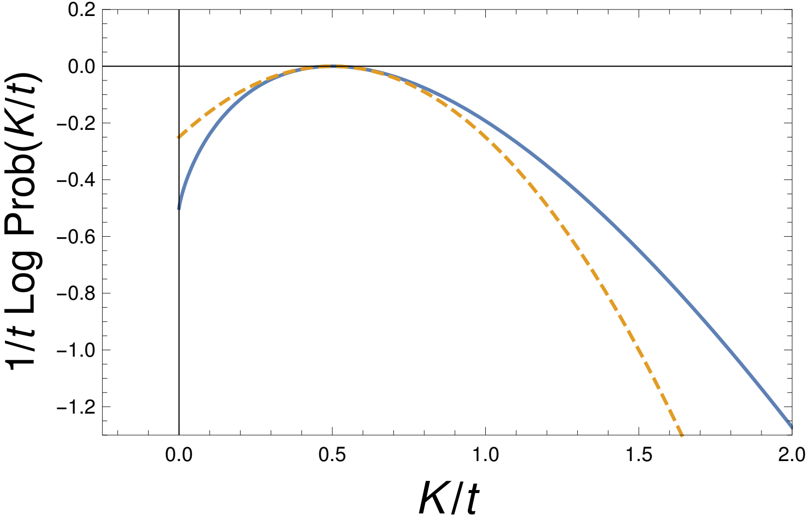
Dashed line: lower noise Continuous line: higher noise

Thanks for your attention!

Supplementary material



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



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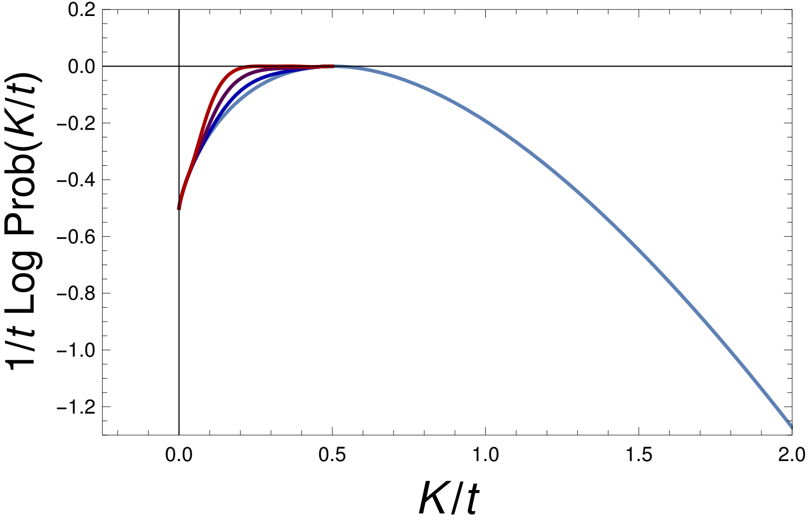

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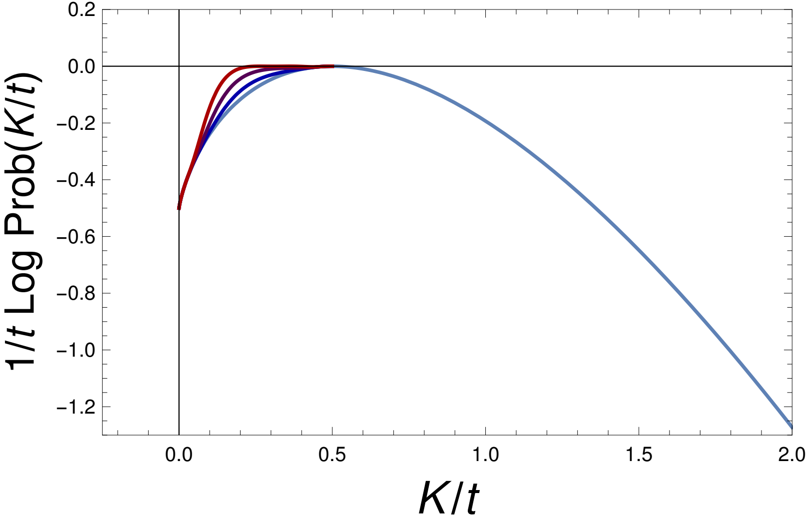
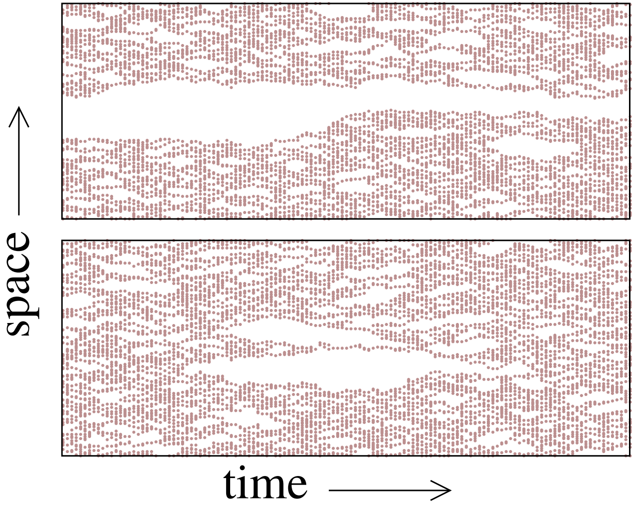
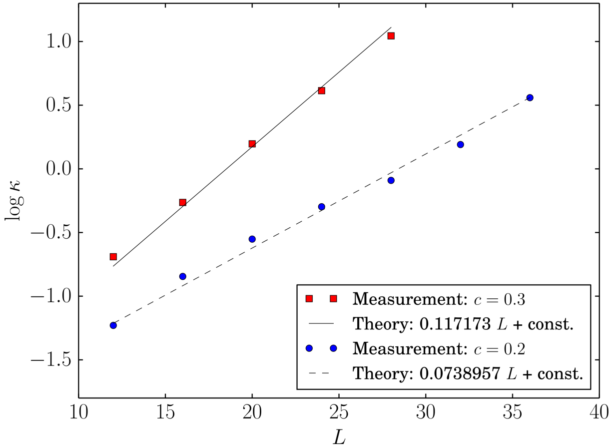


$\text{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.

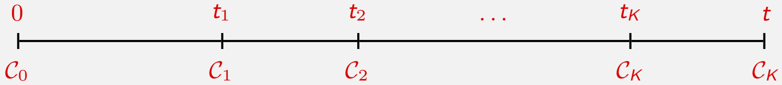


[Merrolle, Garrahan and Chandler, 2005]



Exponential divergence of the susceptibility

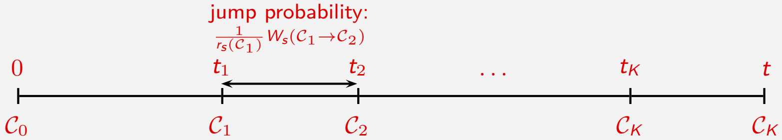
Explicit construction (1/3)



Probability-preserving contribution

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

Explicit construction (1/3)



Which configurations will be visited?

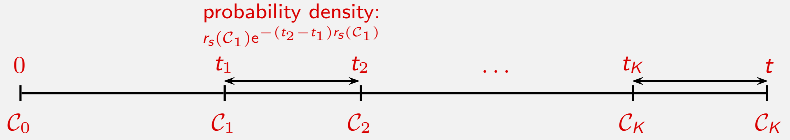
Configurational part of the trajectory: $\mathcal{C}_0 \to \dots \to \mathcal{C}_K$

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

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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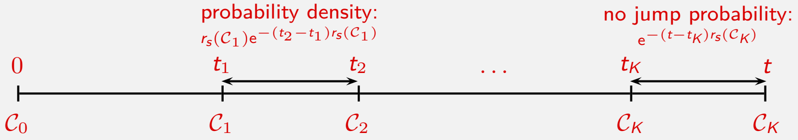

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- probability not to leave $\mathcal{C}_K$ during the time interval $t - t_K$

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

Explicit construction (3/3)

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

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 Δt 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 δr_s $\equiv$ **selection** rendering atypical histories typical