# Large deviations and population dynamics

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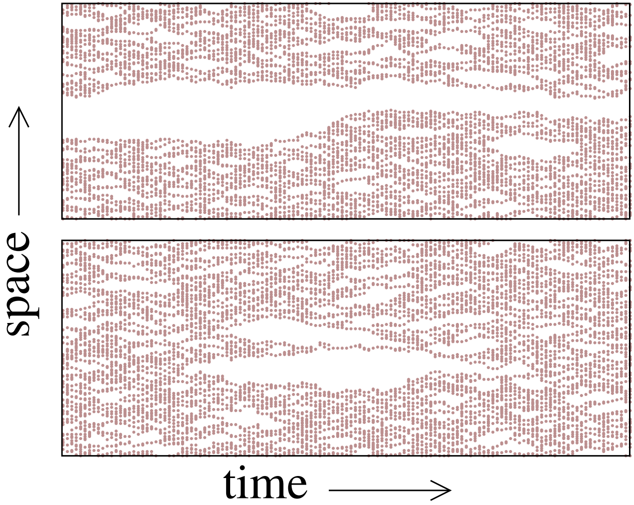
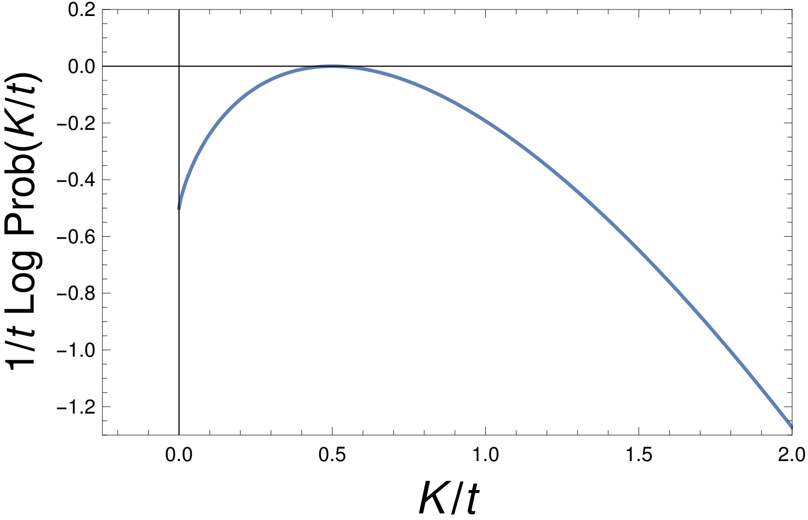
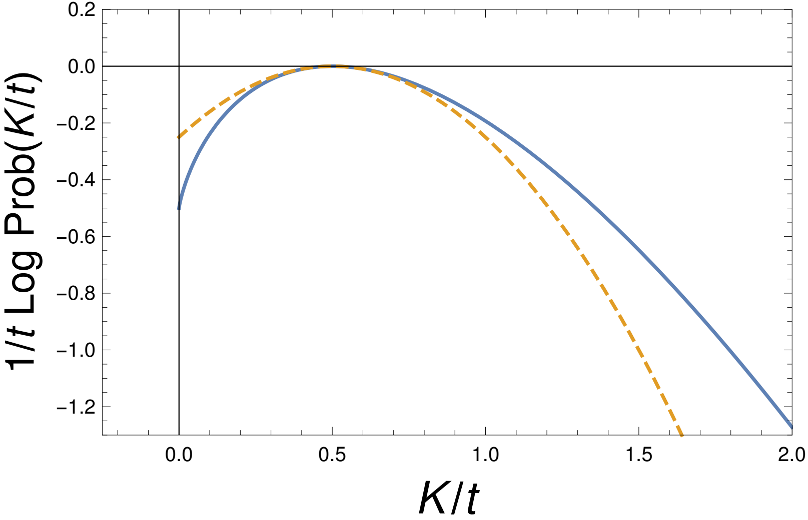



[Merrolle, Garrahan and Chandler, 2005]




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

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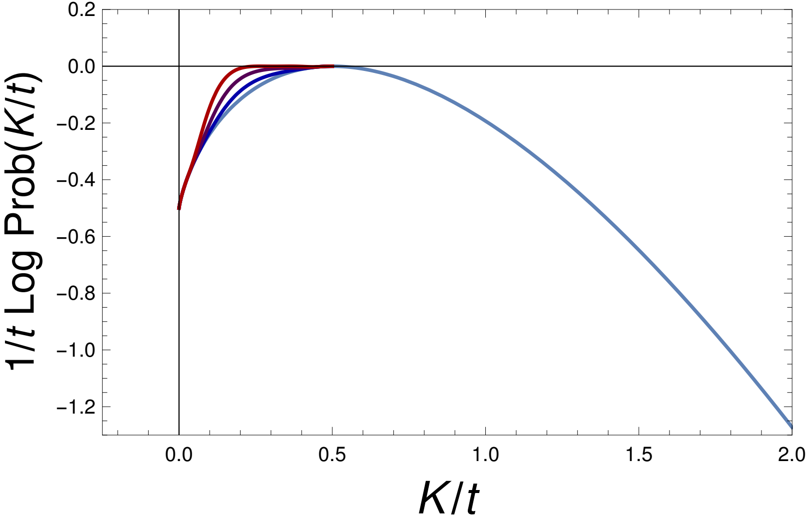


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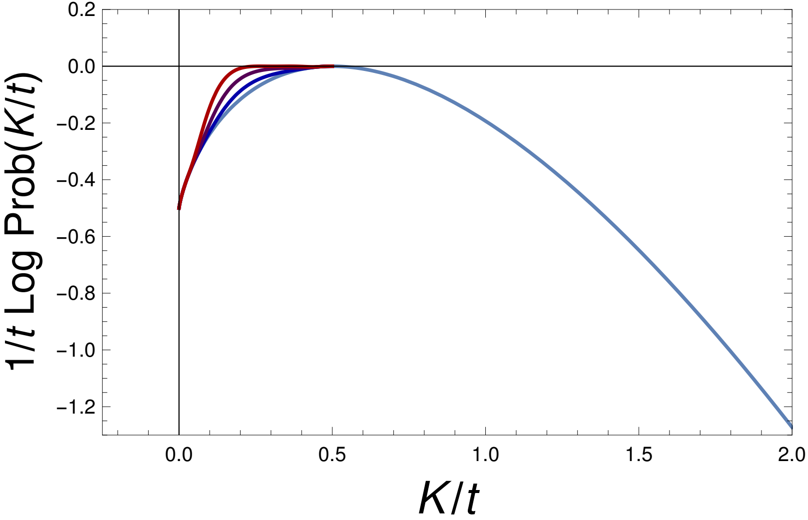


$\text{Prob}[K] \sim e^{t\,\varphi(K/t)}$ Finite-time & -size scalings matter.

# *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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- More detailed dynamics for $P(\mathcal{C},K,t)$:

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$$\partial_t \hat{P}(\mathcal{C},s,t) = \sum_{\mathcal{C}'} \Big\{ \mathrm{e}^{-s} W(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}',s,t) - W(\mathcal{C} \to \mathcal{C}') \hat{P}(\mathcal{C},s,t) \Big\}$$

# Numerical method [with J. Tailleur]

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

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

- 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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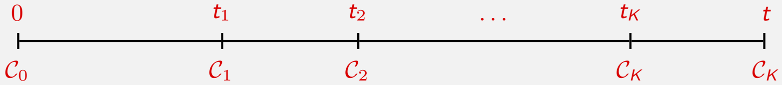
# Explicit construction (1/3)




## Probability-preserving contribution

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

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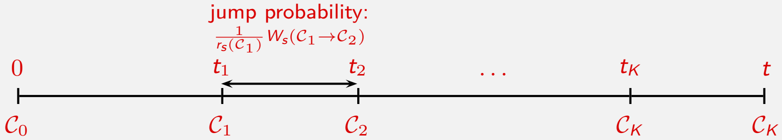



## Which configurations will be visited?

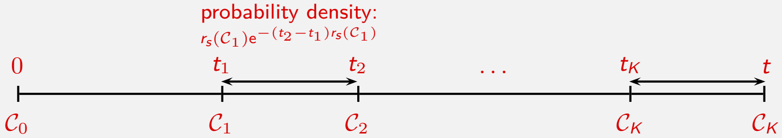
Configurational part of the trajectory: $\mathcal{C}_0 \to \dots \to \mathcal{C}_K$

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

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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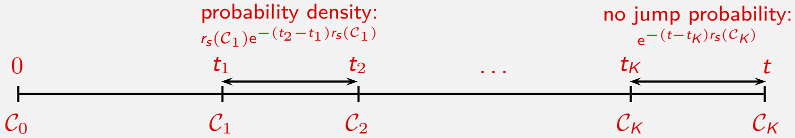


**When shall the system jump from one configuration to the next one?**

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

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

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

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

# Explicit construction (3/3)

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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 un-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

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

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

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

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$$\langle N_{\rm nc}(\mathcal{C},t)\rangle_s = \langle \mathcal{C}|e^{t\mathbb{W}_s}|P_{\rm i}\rangle N_0 \underset{t\to\infty}{\sim} e^{t\psi(s)}\langle \mathcal{C}|R\rangle\langle L|P_{\rm i}\rangle N_0$$

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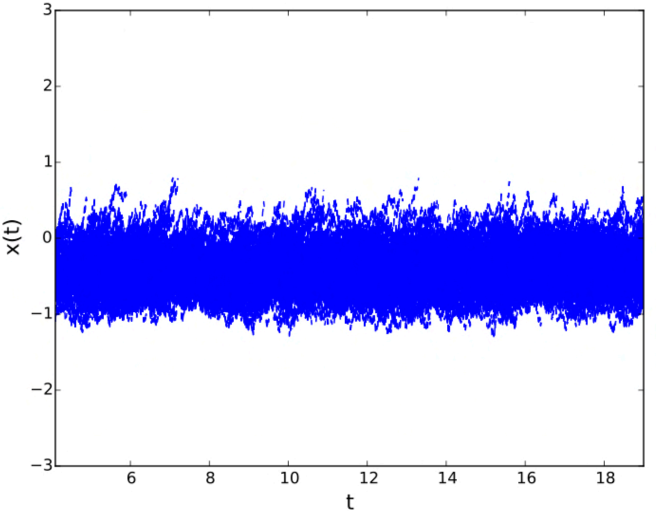
[$N_{\rm nc}$ = number in non-constant population dynamics]

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


3
2
1
0
−1
−2
−3
x(t)
6
8
10
12
14
16
18
t

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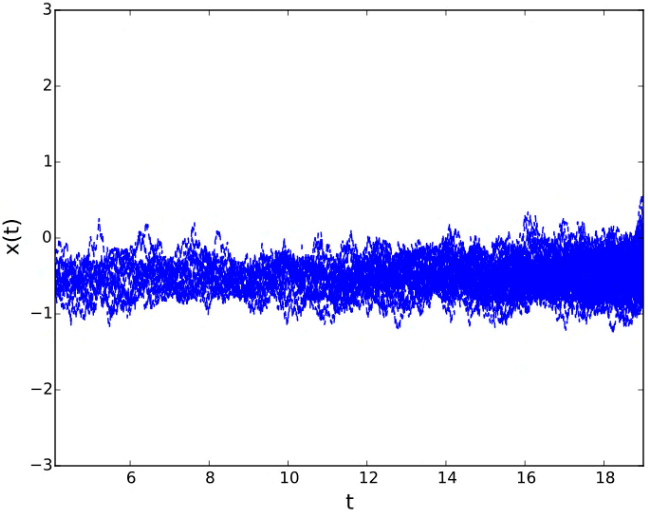
Mid-time distribution governed by **left** and **right** eigenvectors.




Huge sampling issue

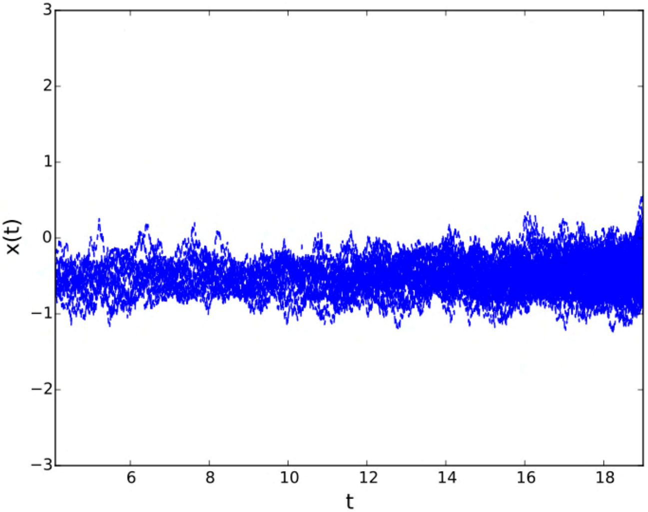
# How to perform averages?

⋆ 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 $t_{\mathrm{f}}$:

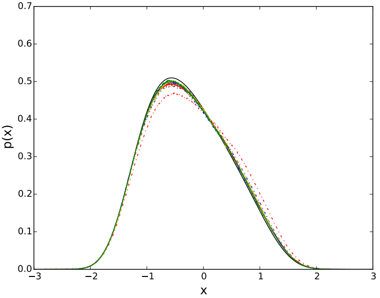
$$p_{\mathrm{anc}}(\mathcal{C}, t_1; \mathcal{C}_{\mathrm{f}}, t_{\mathrm{f}}) = \frac{\langle N_{\mathrm{nc}}(\mathcal{C}_{\mathrm{f}}, t_{\mathrm{f}} | \mathcal{C}, t_1) \rangle_s}{\sum_{\mathcal{C}'} \langle N_{\mathrm{nc}}(\mathcal{C}_{\mathrm{f}}, t_{\mathrm{f}} | \mathcal{C}', t_1) \rangle_s} \underset{t_{\mathrm{f},1}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

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

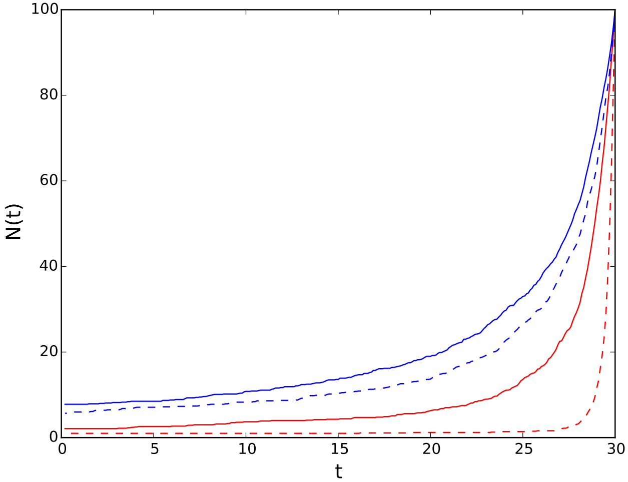



Still huge sampling issue

# Example distributions for a simple Langevin dynamics




$p_{\text{end}}(x)$ $p_{\text{ave}}(x)$




Decrease of the number $N(t)$ of surviving trajectories on $[t_f - t, t_f]$

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

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

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

- Whichever $L_{\text{test}}$, the simulation is still correct.

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

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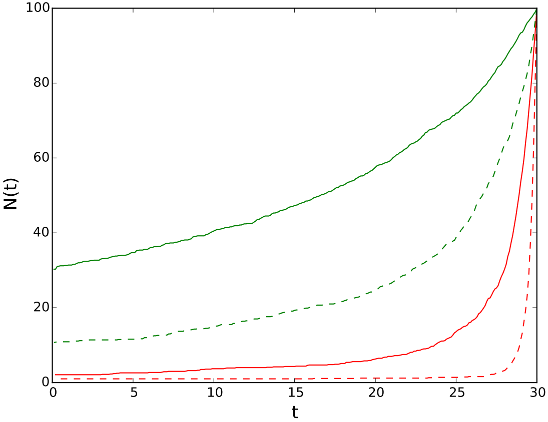
- Whichever $L_{\text{test}}$, the simulation is still correct.

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

Improvement of the depletion-of-ancestors problem:

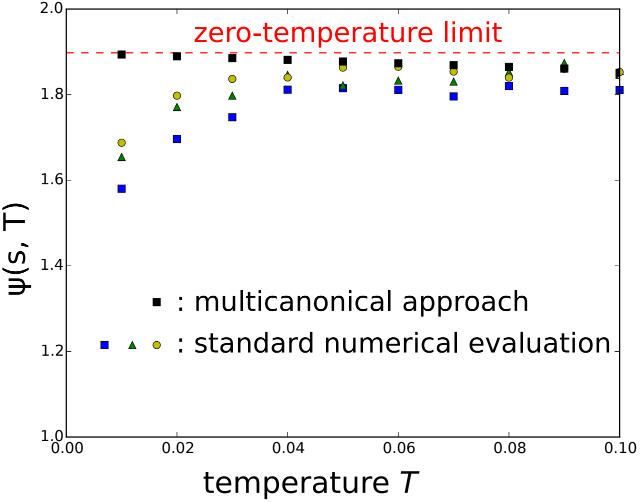



Red: without multicanonical sampling.

Green: with multicanonical sampling ($L_{\text{test}}$ evaluated on the fly)

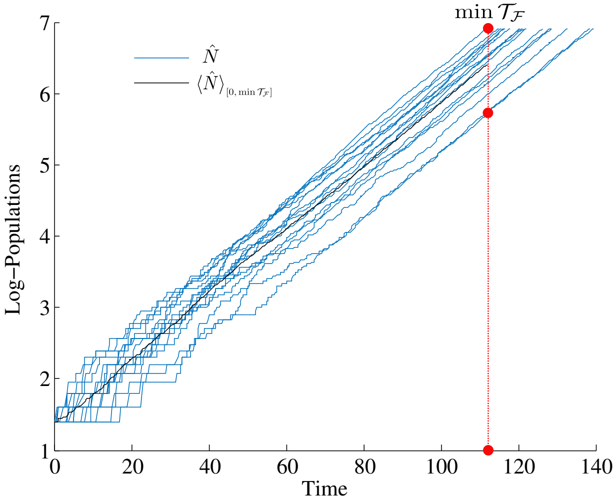
Dashed: lower temperature

Improvement of the small-noise crisis:

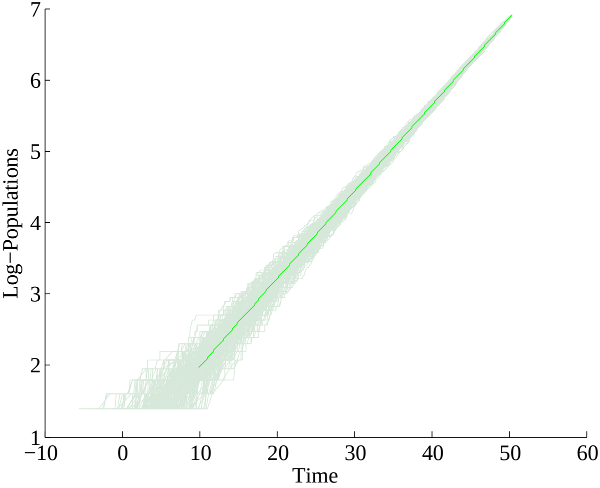


# Initial transient regime [with E. Guevara]

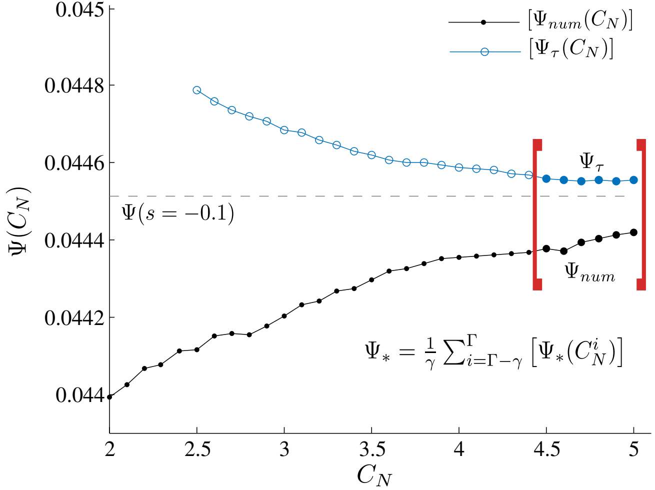
Non-constant population dynamics



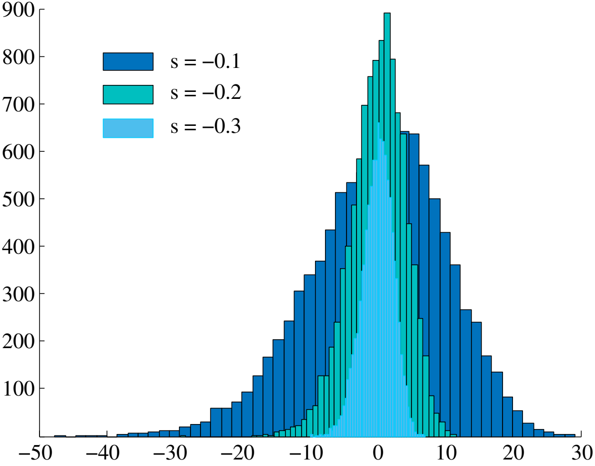
# Time-delay



# Improvement of the numerical evaluation of $\psi(s)$



# Distribution of time delays



# Summary and questions

**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?

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- On-the-fly evaluated auxiliary dynamics
- Solution to the small-noise crisis
- Systems with large number of degrees of freedom?

## Non-constant population dynamics [with E Guevara]

- Sampling problem (depletion of ancestors)
- Initial transient regime due to small population
- Procedure: time-delay
- Analogy with biology: many small islands *vs.* few large islands?