Growing clusters

simple models, symmetry breaking, and fluctuations

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Growth workshop, Nov 2019

Thanks to:
Steve Whitelam, Katie Klymko (Berkeley Lab)
Rosemary Harris (Queen Mary, London)

Something about me...

Theoretical physicist, currently with a joint appointment between Chemistry and Applied Mathematics

[before that, faculty post at Dept of Physics, Bath Uni]

Main interests:

Statistical mechanics
(physical systems with many interacting particles)

Rare events in physics and chemistry

Soft matter, biomolecular physics, self-assembly, ...

Glassy materials

Today

Very simple model for a growing cluster with two kinds of particle

Spontaneous symmetry breaking / "de-mixing"

Analysis of (complex) fluctuations of cluster composition

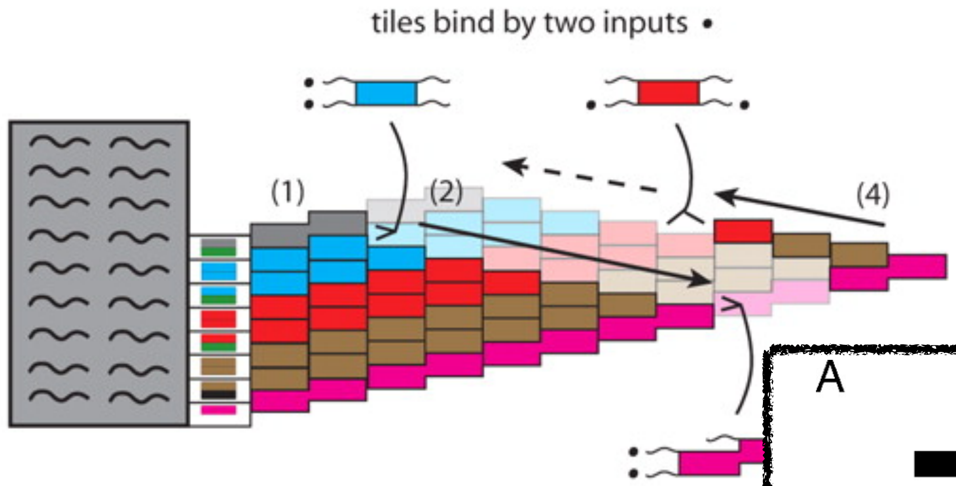
Rare events with non-typical composition in large clusters

Mechanisms for rare events, and strategies for controlling the observed behaviour

[Illustration of research questions and methods]

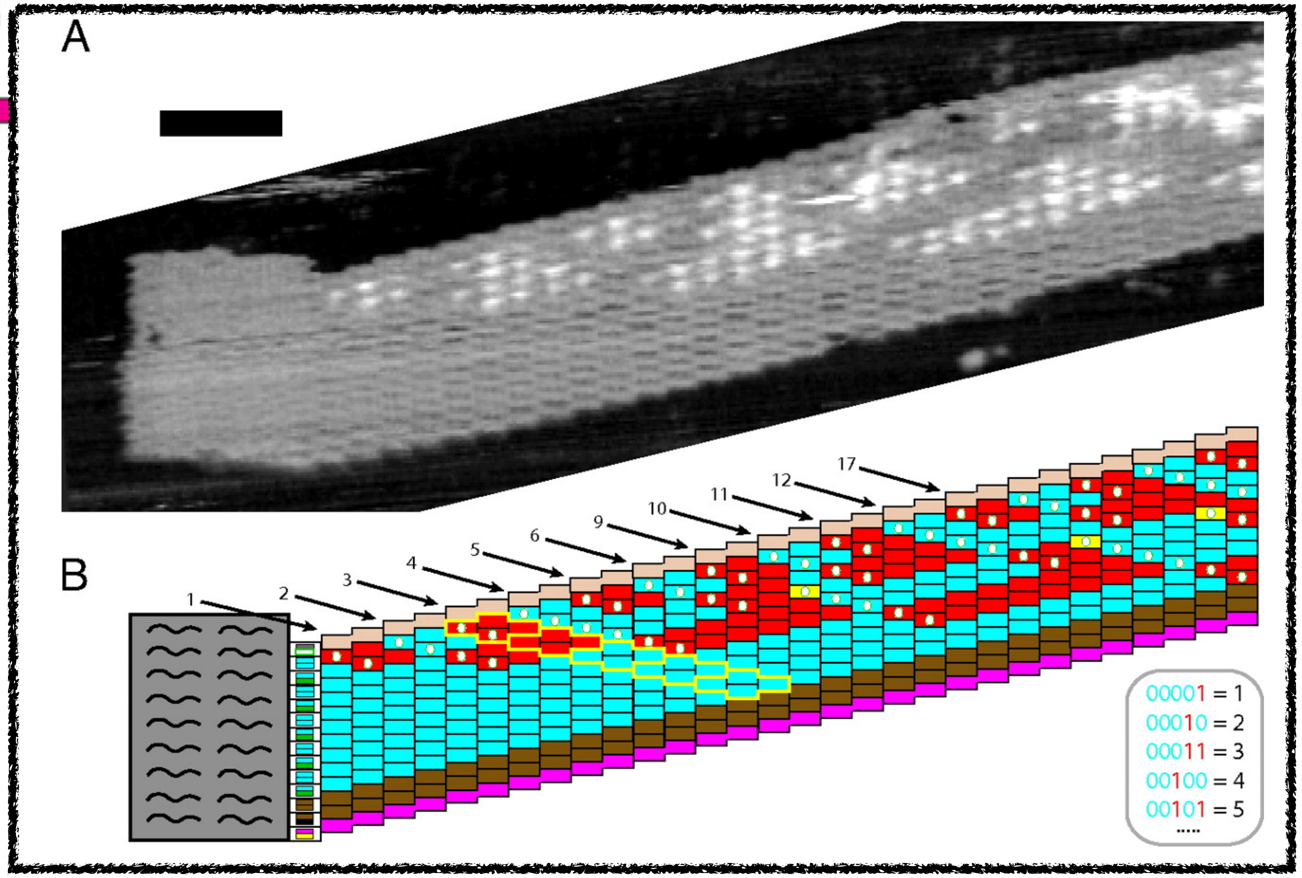
Motivation (i)

[Barish-Schulman-Rothemund-Winfree, PNAS 106, 6054 (2009)]



Idea: use small synthetic pieces of DNA to grow ordered nano-structures ("origami")

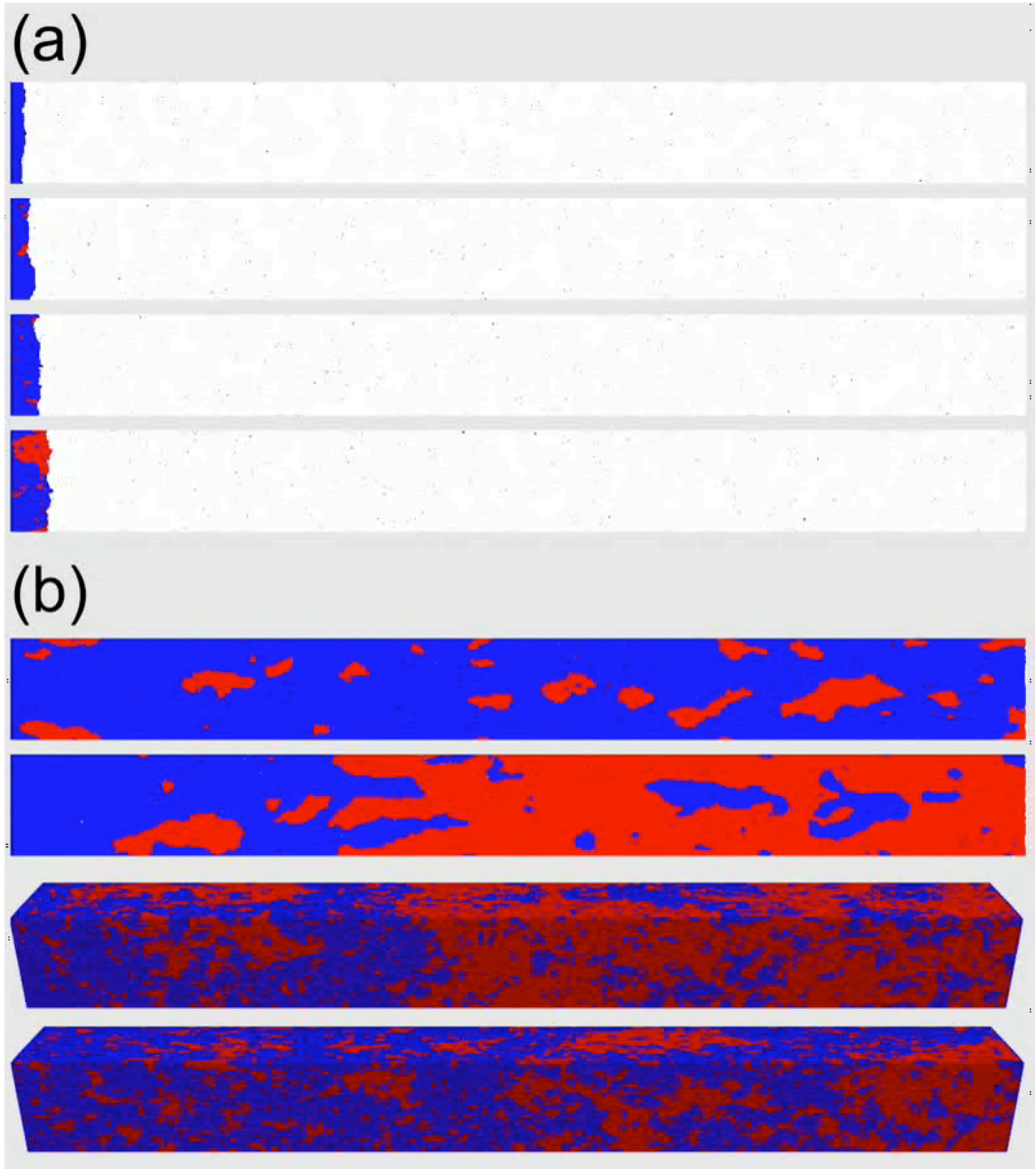
"Algorithmic crystal"



Experiments: scale bar 50nm

Motivation (ii)

[Whitelam-Haxton-Schmidt, Phys Rev Lett 112, 155504 (2014)]



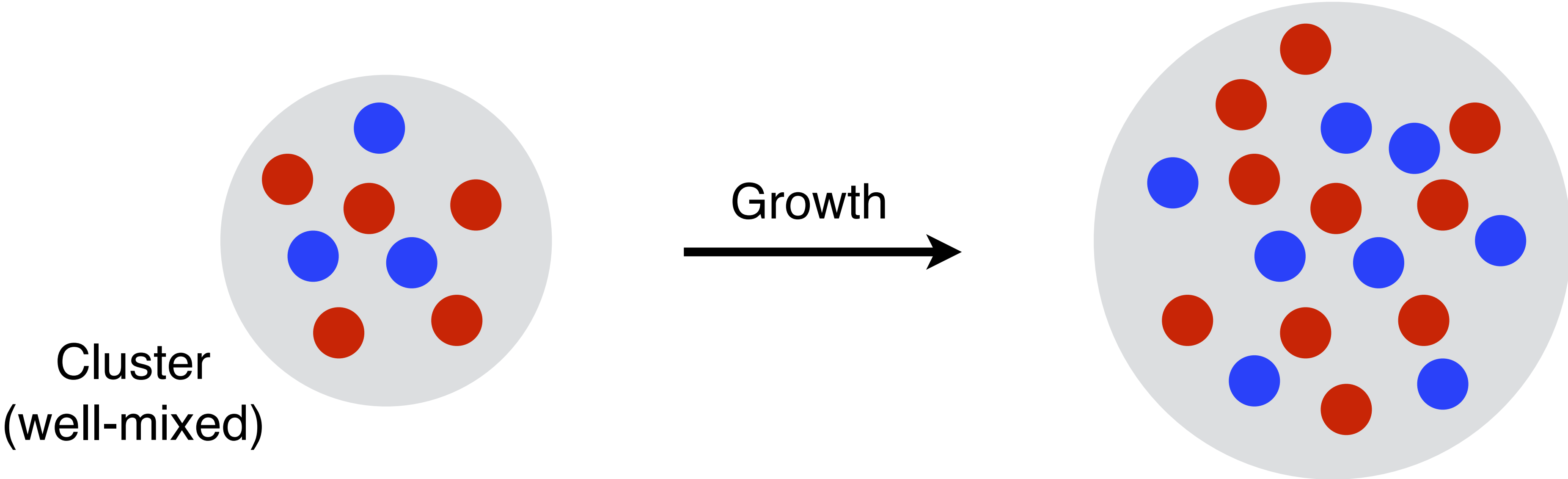
(slow)

(fast)

How to predict "patterns" in systems with growth fronts?

[also Morris-Rogers, J. Phys. A 47, 342003 (2014)]

Simple model



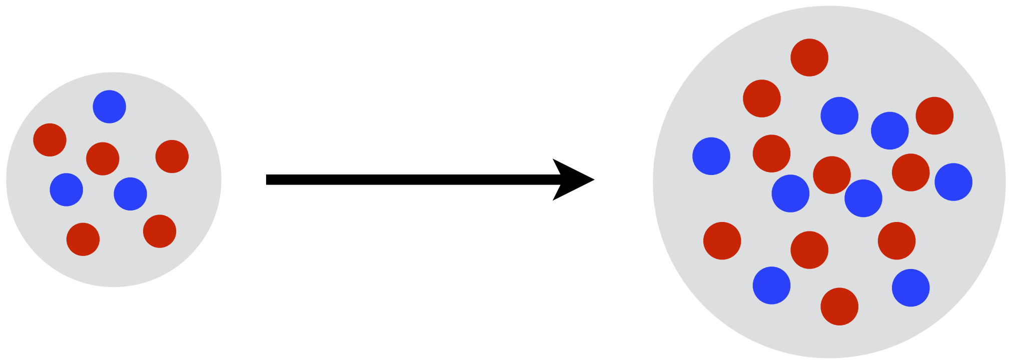
Particles are added, one at a time

If the cluster has K particles then its composition is $m_K = \frac{N_{\mathrm{red}} - N_{\mathrm{blue}}}{K}$, this is between -1 and $+1$

If the cluster is mostly red (large m) it tends to recruit more red particles, and vice versa. The strength of this effect is controlled by a parameter J.

[Klymko-Garrahan-Whitelam, Phys Rev E 96, 042126 (2017)]

Model

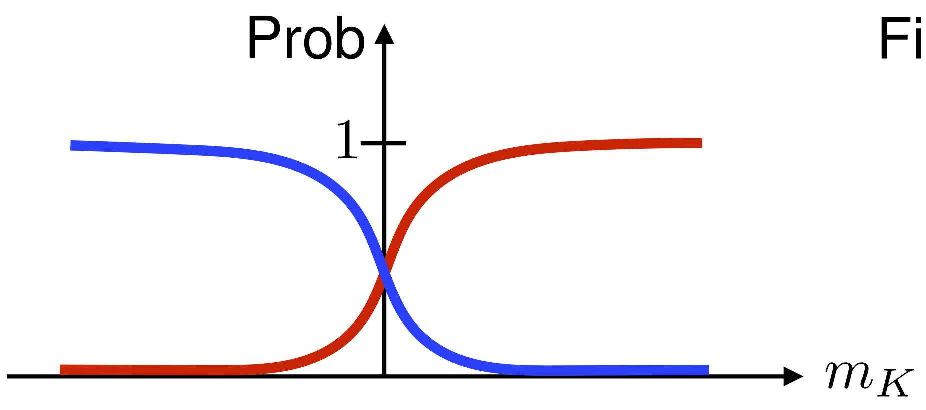


[Klymko, Garrahan, Whitelam, Phys Rev E **96**, 042126 (2017)]

Specifically, on step K the cluster has K particles and composition m_K.

We add:

red particle	with probability $\frac{1}{2}(1 + \tanh Jm_K)$
blue particle	with probability $\frac{1}{2}(1 - \tanh Jm_K)$



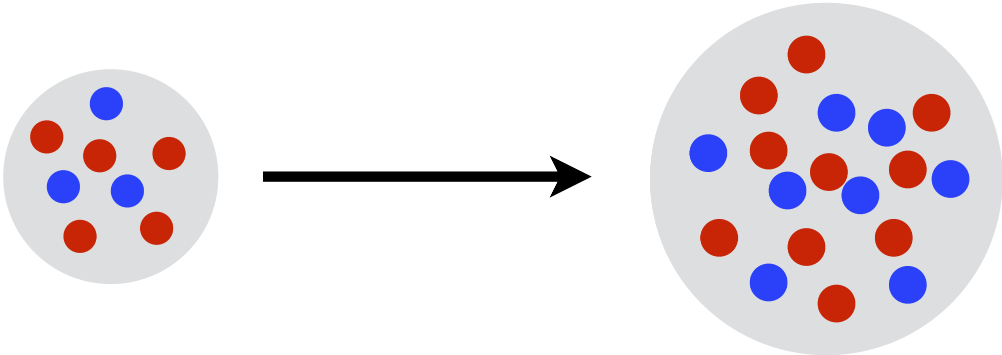
First particle : Prob (1/2)

(Nothing about spatial structure...)

[Polya urn...]

Behaviour

[Klymko, Garrahan, Whitelam,
Phys Rev E **96**, 042126 (2017)]

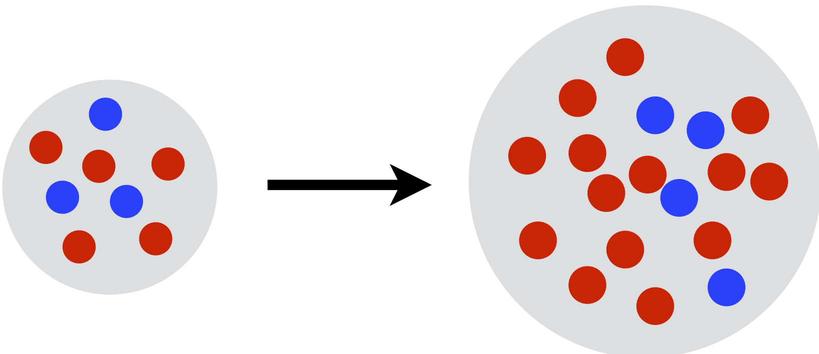


The model is symmetrical between red and blue

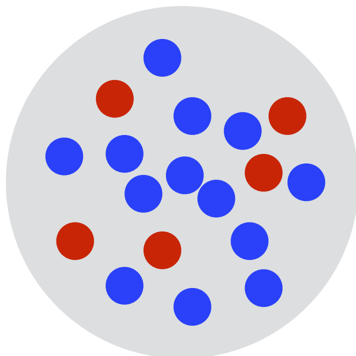
For $J = 0$ then particles are added with random colours

After a large number of steps then $m_K \approx 0$ with (small) standard deviation $\sqrt{1/K}$ ($\ldots$binomial)

For $J > 1$ and large times then one typically finds either $m_K \approx m^*$ or $m_K \approx -m^*$, with equal probability.



or



"Spontaneous symmetry breaking"
or
"de-mixing"

Intuition from continuous time

For intuition, define a model in continuous time, let $M_t = N_{\mathrm{red}} - N_{\mathrm{blue}}$

$$\frac{\mathrm{d}}{\mathrm{d}t} M_t = \tanh(J M_t / t) + (\text{noise})$$

SDE / Langevin

We consider $m_t = M_t / t$, it follows

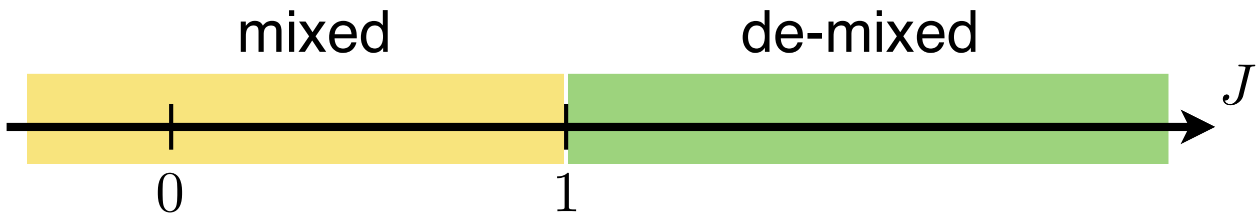
$$\frac{\mathrm{d}}{\mathrm{d}t} m_t = \frac{1}{t} \left[\tanh(J m_t) - m_t + (\text{noise})\right]$$

Fixed points solve $m = \tanh Jm$, noise is weak at large times

Rescaling time as $u = \log t$, we have (for Gaussian noise)

$$\frac{\mathrm{d}}{\mathrm{d}u} m_u = \tanh(J m_u) - m_u + \mathrm{e}^{-u/2} (\text{noise})$$

Summary



[similar behaviour also demonstrated for models with "reversible" growth]

[Klymko, Garrahan, Whitelam,
Phys Rev E **96**, 042126 (2017)]

Questions:

This is the typical behaviour, what about the variance?

central limit theorems

For $J > 1$, we sometimes see mixed clusters, how rare is this?

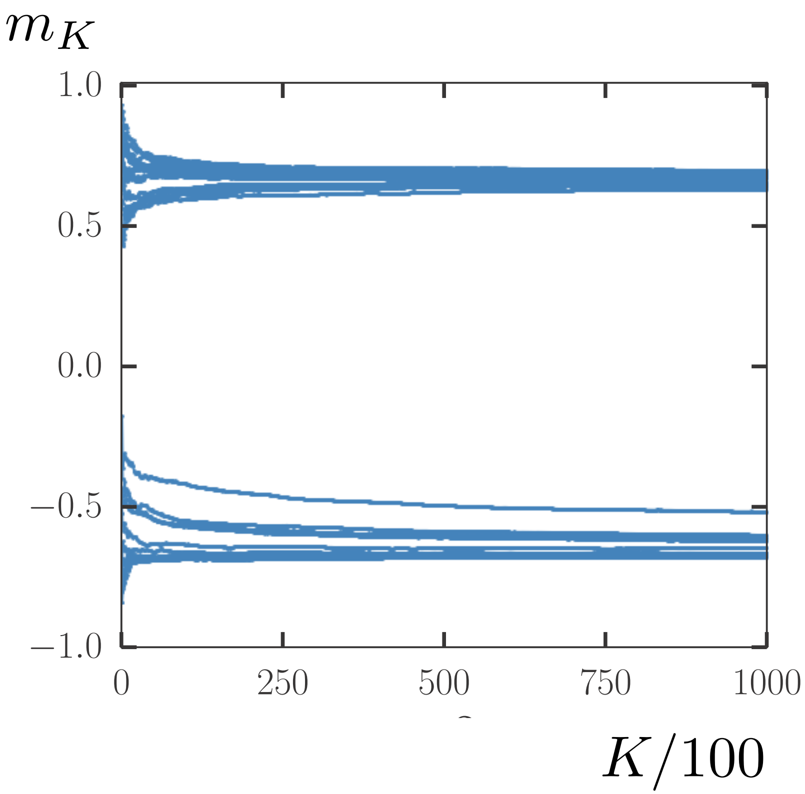
(similarly, do we ever see de-mixed clusters for $J < 1$?)

large deviations...

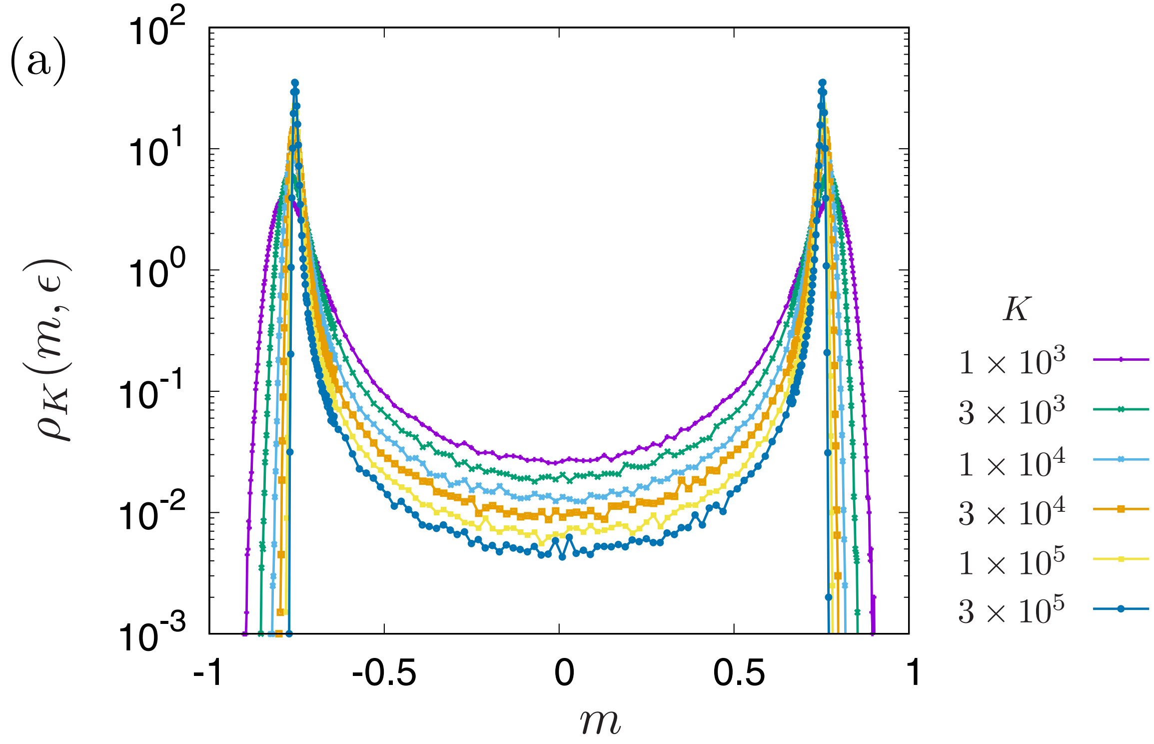
Are there efficient ways to modify system behaviour?
(not simply changing J)

[Klymko, Garrahan, Geissler, Whitelam, Phys Rev E **97**, 032123 (2018),
RLJ, Phys Rev E **100**, 012140 (2019).]

Illustrative results



Trajectories / histories / sample paths for $J = 1.5$



Probability distribution (histograms), for $J = 1.3$

Sharp peaks, broad "trough"

[Klymko, Garrahan, Geissler, Whitelam, Phys Rev E **97**, 032123 (2018)]

[RLJ, Phys Rev E **100**, 012140 (2019)]

Optimal control theory for rare events

[Dupuis-Ellis, etc]

We want to know about unusual behaviour which happens only rarely...

To analyse this, we modify the model so that *the unusual behaviour becomes typical*

In this way we can show that (roughly-speaking)

$$\mathrm{Prob}(\text{rare event}) \gtrsim \exp\left[-\mathcal{D}_{\mathrm{KL}}(\text{new model} \parallel \text{old model})\right]$$

where $\mathcal{D}_{\mathrm{KL}}$ is called Kullback-Leibler divergence.

("at least as likely as...")

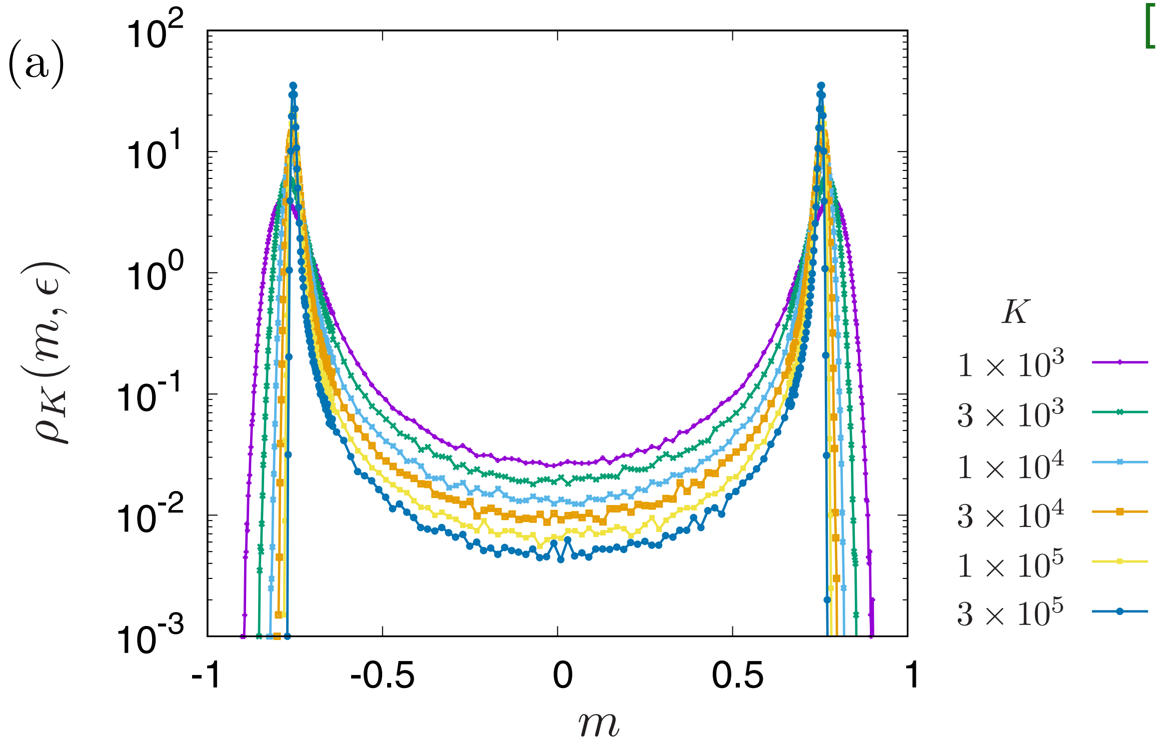
The KL divergence is small if we didn't modify the model too much

The best choice of new model ("optimally controlled model") gives a good estimate of the log-probability of interest. Can take something like

$$\frac{\mathrm{d}}{\mathrm{d}t} m_t = b(t) + \frac{1}{t}(\mathrm{noise})$$

Illustrative results

[RLJ, Phys Rev E **100**, 012140 (2019).]



Peaks are at $\pm m^*$

Trough: less de-mixing than expected

Fluctuations with $|m| > m^*$ have very small probabilities,

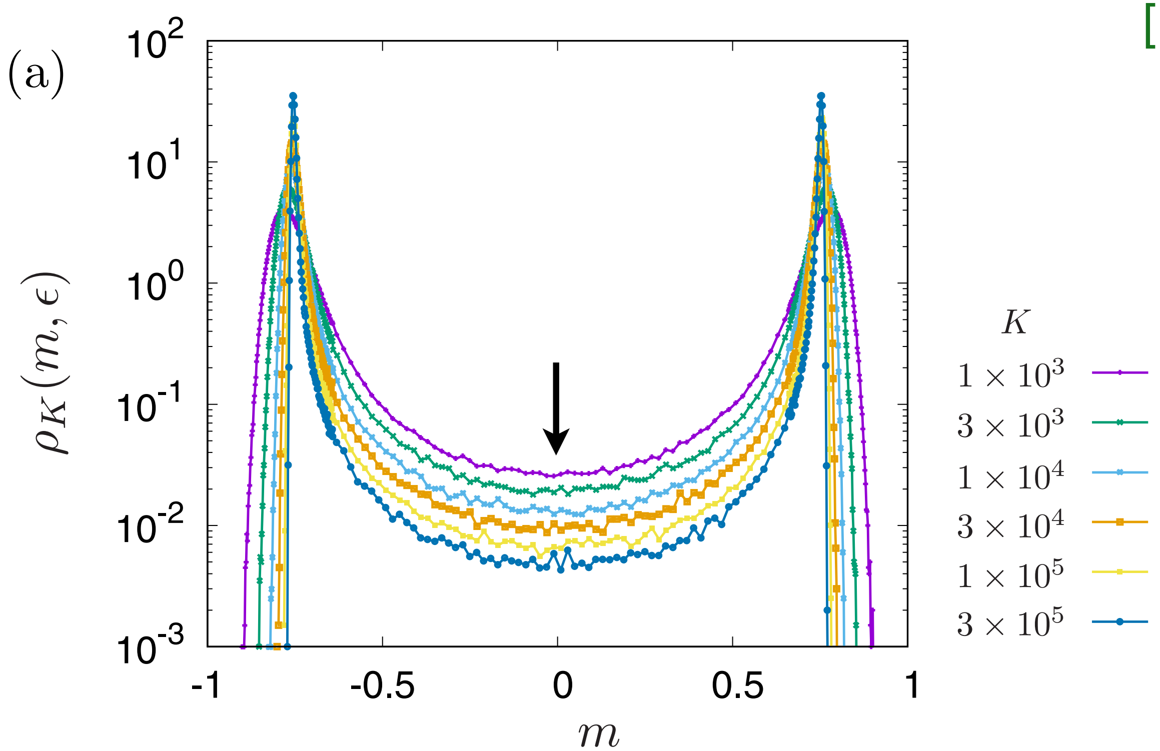
$$-\log p_K(m) \approx I(m)K$$

Fluctuations with $|m| < m^*$ have moderately small probabilities,

$$-\log p_K(m) \approx f(m) \log K + g(m)$$

Controlled process (i)

[RLJ, Phys Rev E **100**, 012140 (2019).]



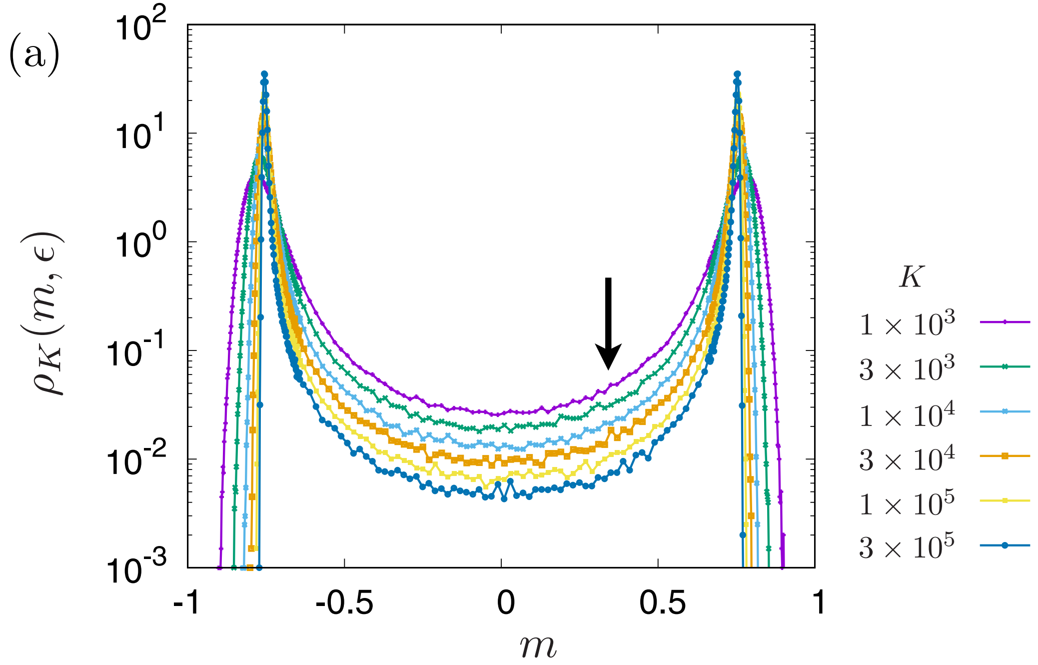
For events with $m_K \approx 0$, the optimally-controlled process stays close to $m_k = 0$ throughout.

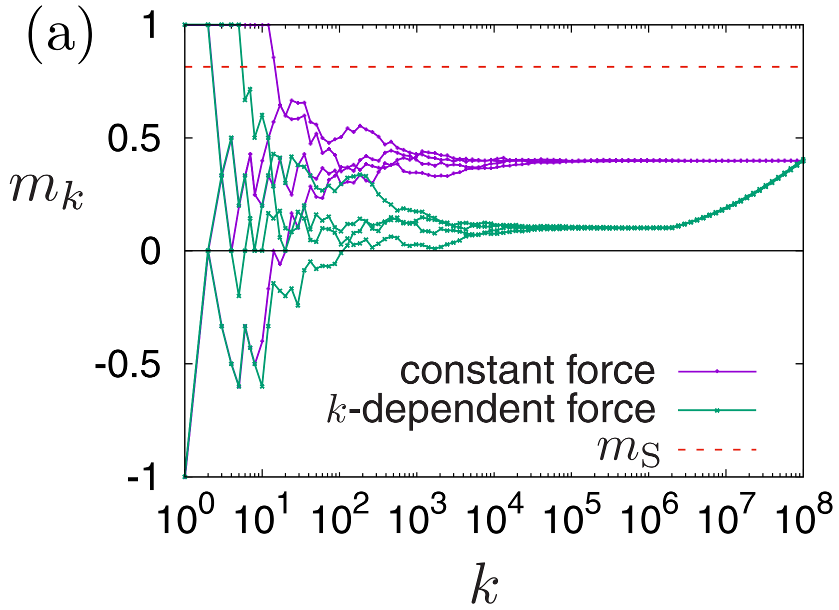
The system “doesn’t know whether to be red or blue”, it turns out that this results in a small KL divergence

We estimate $p_K(0) \simeq cK^{-\frac{J^2(J-1)}{2J-1}}$

Controlled process (ii)

[RLJ, Phys Rev E **100**, 012140 (2019).]



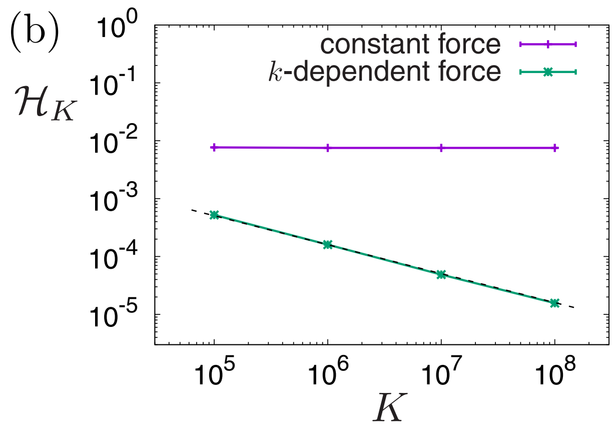


For m_K between 0 and m^*, can consider two different controlled processes:

(i) Stay near the final value m_K throughout

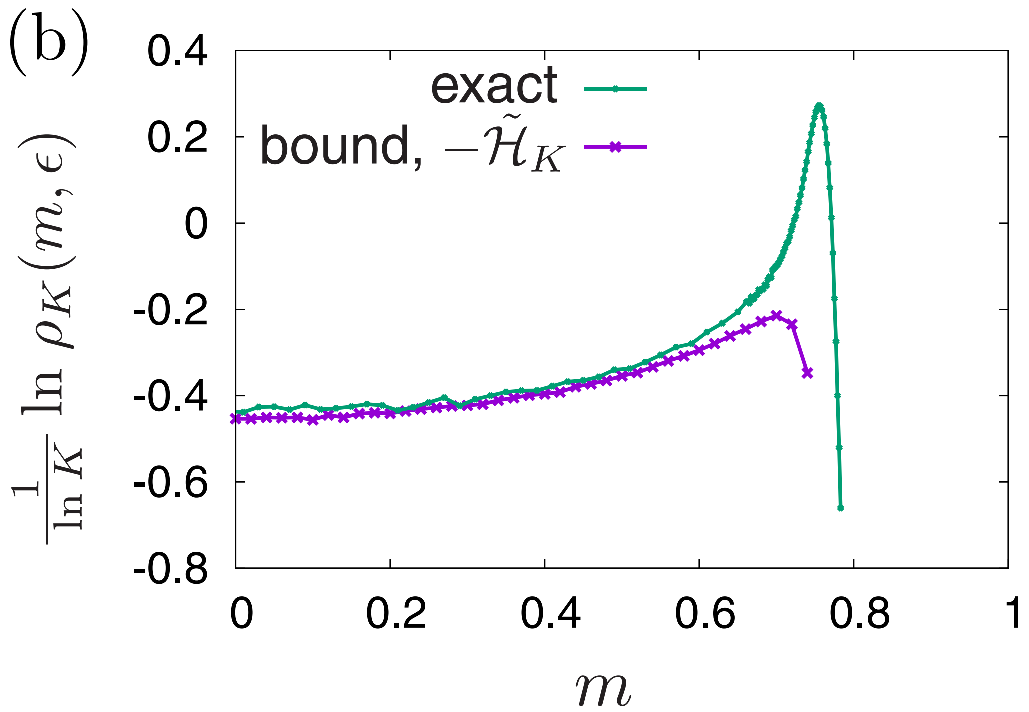
(ii) Start near $m \approx 0$ and de-mix only at late times

In fact (ii) is much closer to optimal



Controlled process (iii)

[RLJ, Phys Rev E **100**, 012140 (2019).]



With a bit more work, we can get a good estimate of the rare-event probability.

Conclusion : the "least unlikely" fluctuation mechanism is "delayed de-mixing".

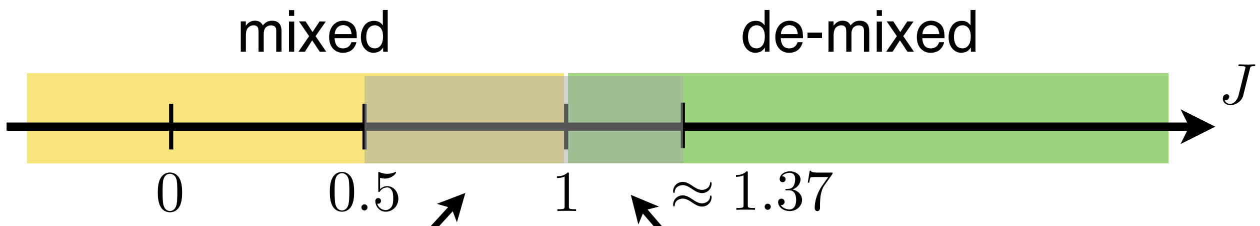
(Use the fact that the system "doesn't know whether to be red or blue" at early times)

[General results for urns, Franchini, Stoch Proc Appl **127**, 3372 (2017)]

[Also: positive feedback for de-mixing, so invest "control budget" at the start]

Other regimes

[RLJ, Phys Rev E **100**, 012140 (2019) + (unpublished),
Franchini, Stoch Proc Appl **127**, 3372 (2017)]



$$-\log p_K(m) \approx I(m)K$$

but no central limit theorem, $I''(m) = 0$

$$\mathrm{Var}(m_K) \propto K^{\alpha}, \qquad \alpha > 1$$

peaks have width $\sim K^{\alpha/2}$
with $\alpha > 1$

Mechanism : make a rare excursion at early times, follow the natural dynamics at late times (generic for positive feedback(?)).

[Harris, J Stat Mech (2015) P07021]

All this behaviour (and more) can be recapitulated in "reversible" growth model

One word on methods

[RLJ, Phys Rev E **100**, 012140 (2019) + (unpublished),
Franchini, Stoch Proc Appl **127**, 3372 (2017)]

The method described so far only gives lower bounds on probabilities

["at least as likely as..."]

In the large-deviation regime [where $\log p_K(m) \approx -KI(m)$] results of Franchini also give upper bounds, using that all rare-event trajectories are similar

[concentration on a single path, following Dupuis-Ellis]

In this case, sufficient to consider biased random walks as controlled processes (but with bias dependent on k, so inhomogeneous).

(optimal path can be found by numerical minimisation)

[see also Harris-Touchette, J Phys A **42**, 342001 (2009);
Harris, J Stat Mech (2015) P07021]

Outlook

Growing systems have interesting fluctuations

One reason is that smaller systems tend to fluctuate more, bigger systems are more robust

Non-typical behaviour at long times originates (in this case) from unusual short-time behaviour, coupled with positive feedback

(generic feature?)

This suggests that growing systems are generically very susceptible to interventions or perturbations at early times...

Simple models can still have surprising behaviour, but (more importantly) a combination of simulation + theory can also be used to study *more realistic + complicated models*