Anomalous scaling in a kinetically constrained model in 1+1 dimensions

Arturo L. Zamorategui.
Modélisation Stochastique

Laboratoire de Probabilités et Modèles Aléatoires.
Supervisor: Vivien Lecomte

June 10, 2014

Goals

1. Understand the *phase coexistence of active-inactive regions* at the point where the *dynamical phase transition* observed in *glassy systems* occurs. Very well captured by KCMs.
2. Determine an *effective model* of the dynamics in the phase transition from the simplest possible model. Is there something simpler that a KCM ?

A glass looks like...

2D binary mixture of hard disks with different radius (*Keys et al* Phys. Rev. X 1, 021013, 2011).

Start movie

Inactive particles vs Active particles

- **Dynamic heterogeneity**: inactive regions with *slow* dynamics and active regions with *fast dynamics*.
- **Facilitated** dynamics: mobility in a region *leads* to motion of neighbouring particles. An *adjacent* excitation is required for both the birth or death of an excitation.

Activity vs Inactivity

Inactive regions surrounded by **active** particles.

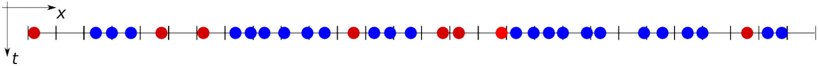
- The *persistent time* (t_p): time a particle remains inactive before the first move.
- The *exchange time* (t_x): time between two consecutive moves. (*Jung et al* 2004).

	Not a glass	**A glass**
Dynamic heterogeneity	$\langle t_p \rangle = \langle t_x \rangle = \tau$	$\langle t_x \rangle \ll \langle t_p \rangle$
Facilitation	-	Particles close to **excitation lines** diffuse more quickly
Stokes-Einstein relations: $D\eta/T =$ constant; $D\tau_\alpha =$ constant; τ_α (relaxation time); D (diffusion coefficient)	Satisfied	Broken, since $\tau_\alpha \approx \langle t_p \rangle$ and $D \approx \delta x^2 / \langle t_x \rangle$: ($D\tau_\alpha \approx \delta x^2 \langle t_p \rangle / \langle t_x \rangle$)

A Kinetically constrained model (KCM)

Dynamic heterogeneity (bubbles of inactivity) and facilitation (excitation lines) are captured by **kinetically constrained models** (KCMs).

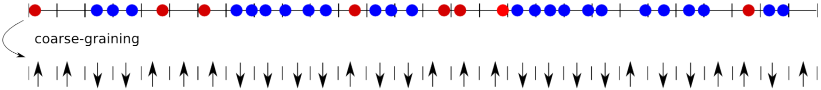
- One spatial dimension (discrete) + one temporal dimension (continuous)



A Kinetically constrained model (KCM)

Dynamic heterogeneity (bubbles of inactivity) and facilitation (excitation lines) are captured by **kinetically constrained models** (KCMs).

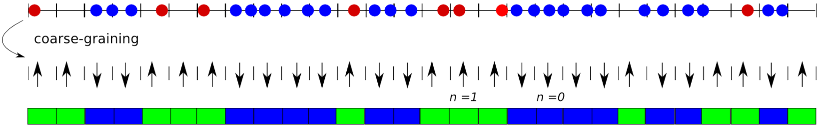
- One spatial dimension (discrete) + one temporal dimension (continuous)
- It is a coarse-grained model with $n_i = 1$ if active and $n_i = 0$ if inactive.



A Kinetically constrained model (KCM)

Dynamic heterogeneity (bubbles of inactivity) and facilitation (excitation lines) are captured by **kinetically constrained models** (KCMs).

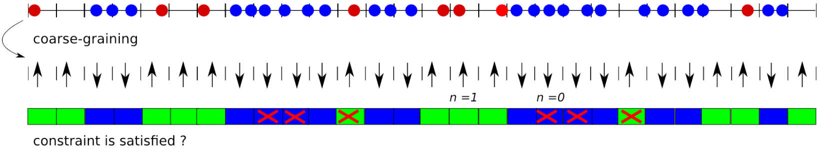
- One spatial dimension (discrete) + one temporal dimension (continuous)
- It is a coarse-grained model with $n_i = 1$ if active and $n_i = 0$ if inactive.



A Kinetically constrained model (KCM)

Dynamic heterogeneity (bubbles of inactivity) and facilitation (excitation lines) are captured by **kinetically constrained models** (KCMs).

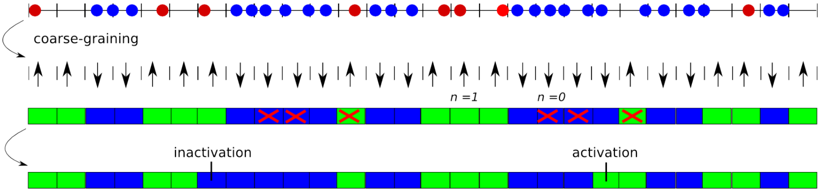
- One spatial dimension (discrete) + one temporal dimension (continuous)
- It is a coarse-grained model with $n_i = 1$ if active and $n_i = 0$ if inactive.
- Dynamic is controlled by a local **constraint**.



A Kinetically constrained model (KCM)

Dynamic heterogeneity (bubbles of inactivity) and facilitation (excitation lines) are captured by **kinetically constrained models** (KCMs).

- One spatial dimension (discrete) + one temporal dimension (continuous)
- It is a coarse-grained model with $n_i = 1$ if active and $n_i = 0$ if inactive.
- Dynamic is controlled by a local **constraint**.



Statics vs Dynamics

- Non-conservative system
- Site i changes state with rate $f_i[(1-c)n_i + c\,(1-n_i)]$, where c is the density of active sites and f_i is the **kinetic constraint**.
- $f_i = 1$ if constraint is satisfied and $f_i = 0$ otherwise.
- f_i depends on the neighbourhood but not on n_i.
- Detailed balanced holds w.r.t Boltzmann distribution (Bernoulli product measure) with energy $\sum_i n_i$ and inverse temperature β ($c = 1/(1+e^{\beta})$).
- Since *statics* is trivial, we need a *dynamical description*.

A dynamic observable: the Activity

Let $\mathcal{C}(t)$ be a configuration of the system at time t. We define a (discrete) **observable** as

$$A[\text{trajectory}] = \sum_{k=1}^{K} \alpha(\mathcal{C}(t_{k-1}) \to \mathcal{C}(t_k)),$$

over K changes of configurations between times 0 and T.

Activity

The **activity** is $K[\text{trajectory}] = \#\text{events}$, i.e. $\alpha(\mathcal{C}(t_{k-1}) \to \mathcal{C}(t_k)) = 1$ when configuration changes.

Evolution of a KCM

The master equation for the evolution of the probability $P(\mathcal{C}, A, t)$ is

$$\frac{\partial P(\mathcal{C}, A, t)}{\partial t} = \sum_{\mathcal{C}'} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', A - \alpha(\mathcal{C}' \to \mathcal{C}), t) - r(\mathcal{C}) P(\mathcal{C}, A, t)$$

having measured a value A of the observable between 0 and t.
$r(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C} \to \mathcal{C}')$ is the escape rate.

Continuous time: at each site there is a clock that changes the state n_i after a time Δt given by $p(\Delta t) = W(n_i \to 1 - n_i) e^{-W(n_i \to 1 - n_i)\Delta t}$.

Large deviation

To have certain dynamics one can *bias* a trajectory according to a parameter s, with trajectory with *lower than normal activity* $(s > 0)$ or *higher than normal activity* $(s < 0)$:

$$P[\text{trajectory}] \rightarrow P_s[\text{trajectory}] = \frac{P[\text{trajectory}]e^{-sK[\text{trajectory}]}}{Z_s},$$

where $Z_s = \langle e^{-sK[\text{trajectory}]} \rangle$.
For large observation times:

$$\lim_{t\rightarrow\infty} \frac{\ln Z_s}{t} \rightarrow \psi_K(s).$$

$\psi_K(s)$ is a **large deviation function**, also known as *dynamical free energy*.

First order phase transition

$\psi_K(s)$ presents a **singularity** at $s = 0$:

- $s < 0$: trajectory where $\langle K_t \rangle$ is larger.
- $s = 0$: trajectory with coexistence of active and inactive regions.
- $s > 0$: trajectory where $\langle K_t \rangle$ is smaller.

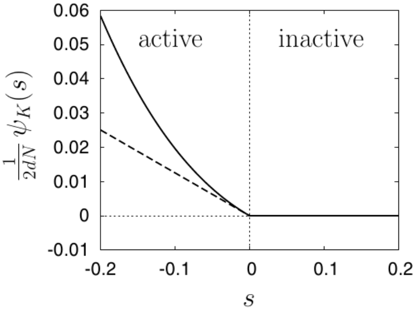


Figure: Active-Inactive transition (Garrahan et al (2007)).

Fredrickson-Andersen Model (FA-1f)

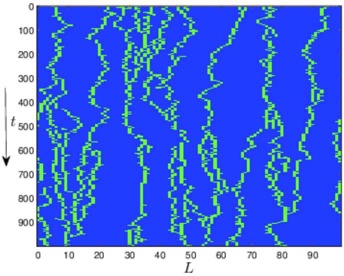
- The transition rates in the FA model are

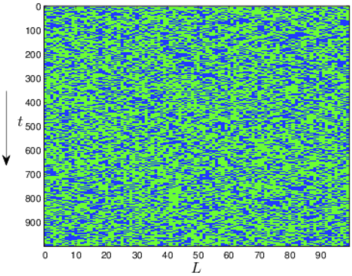
$$W(n_i \to 1 - n_i) = f_i(n_j)\frac{e^{\beta(n_i-1)}}{1+e^{-\beta}},$$

  where $f_i = 1$ if $\sum_{j\sim i} n_j > 0$, i.e if there is *at least one* active site in the neighbourhood, otherwise $f_i = 0$.
- For an **activation**: $W(0 \to 1) = f_i \frac{1}{1+e^{\beta}}$. the term $c = 1/(1+e^{\beta})$ is the *density of active sites*.
- Mean distance between excitations: $l = 1/c$

Typical histories (with $s = 0$) for different densities

Histories of length $L = 100$ and $t = 1000$ for $c = 0.1$ and 0.6.



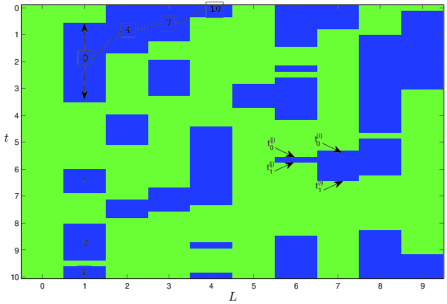


Part 1

Describe bubbles of inactivity

There is not an effective model to understand the **phase coexistence of activity and inactivity** which is generic in glasses.

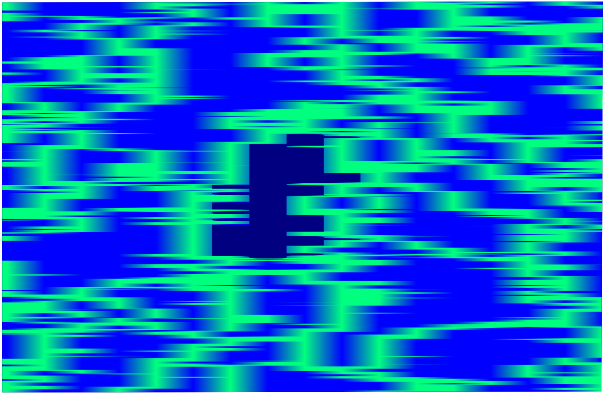
Such a model must describe how bubbles of inactivity evolve in space-time .



1. *Order columns* of inactivity
2. Columns → Nodes
3. Build *adjacency* matrix (from overlap of nodes)
4. *Find bubbles* by identifying one node, its neighbours,...

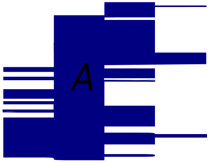
Statistics on bubbles

Focus on one bubble...

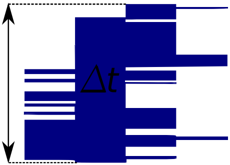


Geometrical Properties

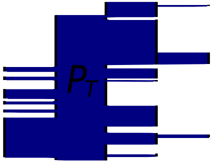
Area



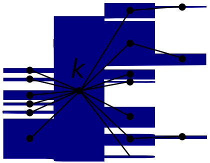
Temporal extension



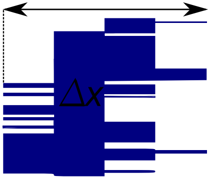
Temporal perimeter



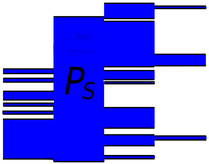
Number of Nodes



Spatial extension

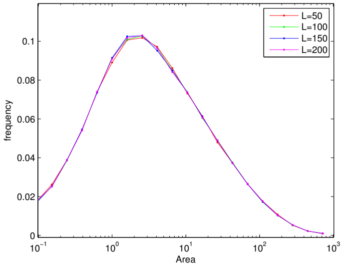


Spatial perimeter



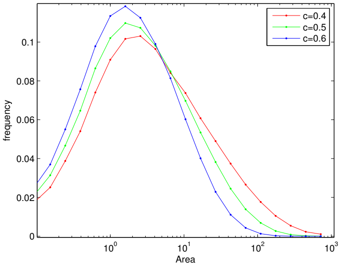
Histograms for the Area

Varying L:



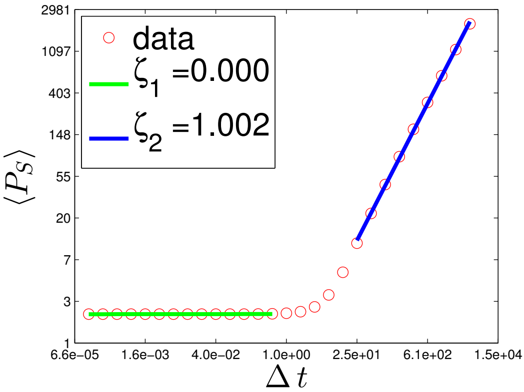
Curves superimpose for different L

Varying c:



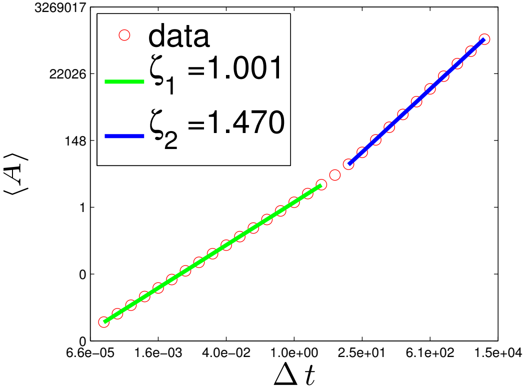
As c decreases, bigger bubbles appear

Spatial Perimeter



$P_S \sim \Delta t^{1.002}$ for large bubbles

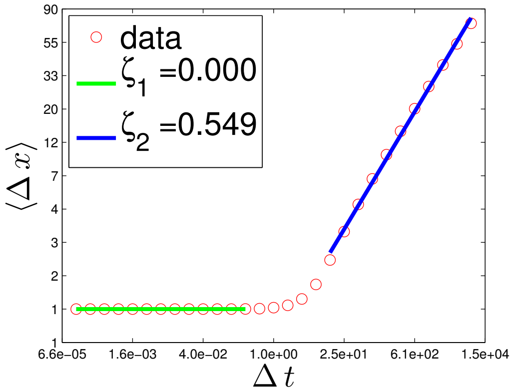
Area



$A \sim \Delta t^{1.470}$ for large bubbles, close to Brownian with $\zeta = 3/2$.*

*S. Majumdar et al. 2005

Spatial extension

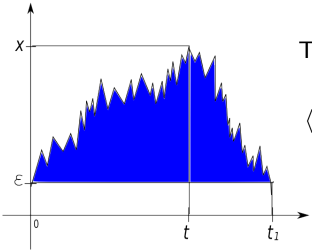


$\Delta x \sim \Delta t^{0.549}$ for large bubbles, bigger than Brownian where $\zeta = 1/2$

Mean shape of bubbles

The probability that r.w. arrives to x_1 at time t_1 given that started at x_0 at time t_0 is:

$$P_\varepsilon(x_1, t_1|x_0, t_0) = \frac{1}{\sqrt{2\pi D(t_1 - t_0)}}\left[e^{\frac{-(x_1-x_0-\varepsilon)^2}{2D(t_1-t_0)}} - e^{\frac{-(x_1-x_0+\varepsilon)^2}{2D(t_1-t_0)}}\right]$$



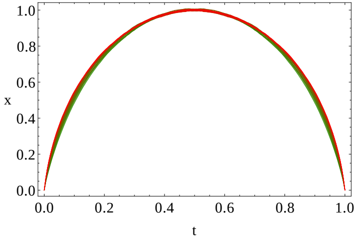
The mean value of $x(t, t_1)$ is:

$$\langle x(t,t_1)\rangle_{[t_0,t_1]} = \frac{\int_0^\infty dx\, x\, P_\varepsilon(x_1,t_1|x,t)P_\varepsilon(x,t|x_0,t_0)}{\int_0^\infty dx P_\varepsilon(x_1,t_1|x,t)P_\varepsilon(x,t|x_0,t_0)}$$

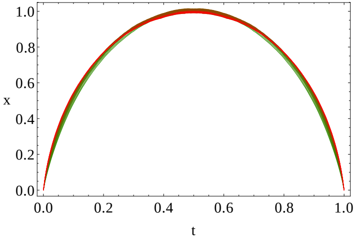
Numerical mean shape

By scaling average curves of bubbles with duration $\Delta t - \varepsilon < \Delta t < \Delta t + \varepsilon$ as $F(\tau) \sim \Delta t^{-\zeta} f(\tau \Delta t)$.

$\zeta = 0.5$:



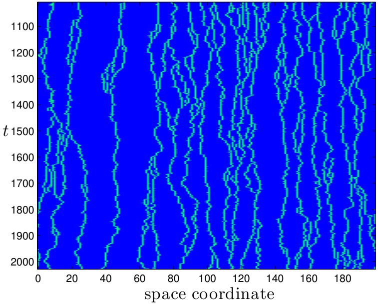
$\zeta = 0.6$:

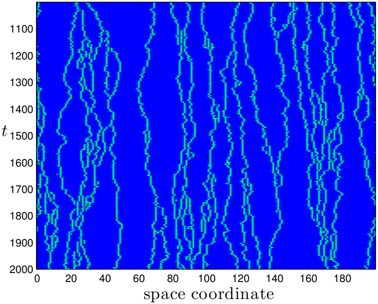


Part 2

FA model for small c

At low temperature (small c) the borders of the bubbles of inactivity in the FA model have some few active sites (left). The dynamics in the FA can be reproduced by a model of branching-coalescence (right) (Whitelan,Berthier,Garrahan 2005).



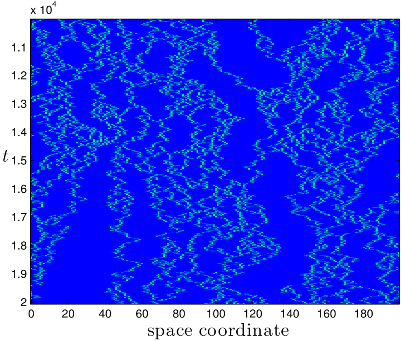


Borders of activity look like random walkers that *branch*, *diffuse* and *coalesce*.

Branching-Coalescing process

We can simulate the system as a branching-coalescing process if

- it captures the same dynamics that the FA model
- Is valid at finite time scales
- Is analytically tractable



Model of branching coalescence

- Initial condition with density c of active sites.

Model of branching coalescence

- Initial condition with density c of active sites.
- A configuration $\mathcal{C}$ changes after a time Δt as $p(\Delta t) = r(\mathcal{C})e^{-r(\mathcal{C})\Delta t}$ where
- the *escape rate* is

$$r(\mathcal{C}) = \sum_i f_i(\mathcal{C})[\underbrace{(1-n_i)c}_{\text{activation}} + \underbrace{n_i(1-c)}_{\text{inactivation}}] = r_{\text{act}}(\mathcal{C}) + r_{\text{inact}}(\mathcal{C})$$

Model of branching coalescence

- Initial condition with density c of active sites.
- A configuration $\mathcal{C}$ changes after a time Δt as $p(\Delta t) = r(\mathcal{C})e^{-r(\mathcal{C})\Delta t}$ where
- the *escape rate* is

$$r(\mathcal{C}) = \sum_i f_i(\mathcal{C})[\underbrace{(1-n_i)c}_{\text{activation}} + \underbrace{n_i(1-c)}_{\text{inactivation}}] = r_{\text{act}}(\mathcal{C}) + r_{\text{inact}}(\mathcal{C})$$

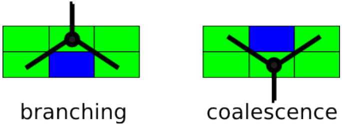
- An **activation** with probability: $p_{\text{act}} = \frac{r_{\text{act}}(\mathcal{C})}{r(\mathcal{C})}$ and an **inactivation** with probability: $p_{\text{inact}} = \frac{r_{\text{inact}}(\mathcal{C})}{r(\mathcal{C})}$.

Model of branching coalescence

- Initial condition with density c of active sites.
- A configuration $\mathcal{C}$ changes after a time Δt as $p(\Delta t) = r(\mathcal{C})e^{-r(\mathcal{C})\Delta t}$ where
- the *escape rate* is

$$r(\mathcal{C}) = \sum_i f_i(\mathcal{C})[\underbrace{(1-n_i)c}_{\text{activation}} + \underbrace{n_i(1-c)}_{\text{inactivation}}] = r_{\text{act}}(\mathcal{C}) + r_{\text{inact}}(\mathcal{C})$$

- An **activation** with probability: $p_{\text{act}} = \frac{r_{\text{act}}(\mathcal{C})}{r(\mathcal{C})}$ and an **inactivation** with probability: $p_{\text{inact}} = \frac{r_{\text{inact}}(\mathcal{C})}{r(\mathcal{C})}$.
- A border of activity constrained to have maximum 3 active sites.

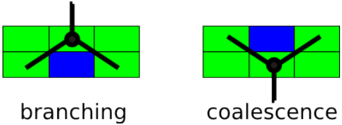


Model of branching coalescence

- Initial condition with density c of active sites.
- A configuration $\mathcal{C}$ changes after a time Δt as $p(\Delta t) = r(\mathcal{C})e^{-r(\mathcal{C})\Delta t}$ where
- the *escape rate* is

$$r(\mathcal{C}) = \sum_i f_i(\mathcal{C})[\underbrace{(1-n_i)c}_{\text{activation}} + \underbrace{n_i(1-c)}_{\text{inactivation}}] = r_{\text{act}}(\mathcal{C}) + r_{\text{inact}}(\mathcal{C})$$

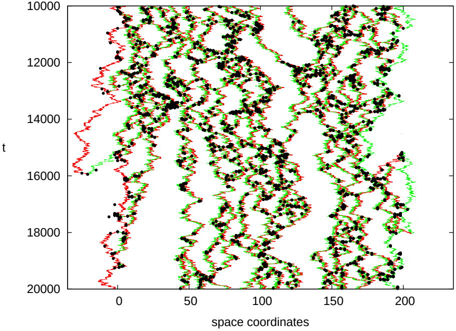
- An **activation** with probability: $p_{\text{act}} = \frac{r_{\text{act}}(\mathcal{C})}{r(\mathcal{C})}$ and an **inactivation** with probability: $p_{\text{inact}} = \frac{r_{\text{inact}}(\mathcal{C})}{r(\mathcal{C})}$.
- A border of activity constrained to have maximum 3 active sites.



Strategy

In *continuous space*: two random walkers will cross an infinite number of times.

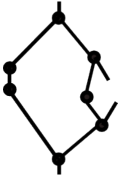
In *discrete space*: is reflected in small bubbles. Focus on branching/coalescing points of large bubbles (of duration $T > 10$)

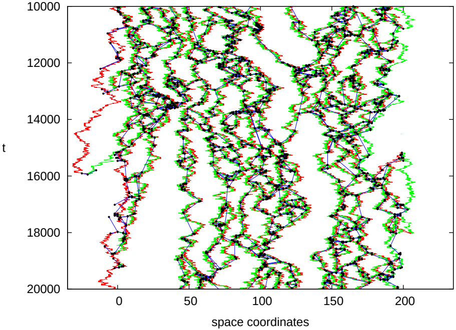


Analysis

The rates are the same by time reversal *symmetry*. How often do we have a branching/coalescing event?

To have just branching and coalescing points we use a **contraction** algorithm until there's no isolated point...

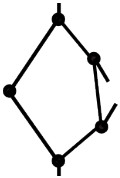


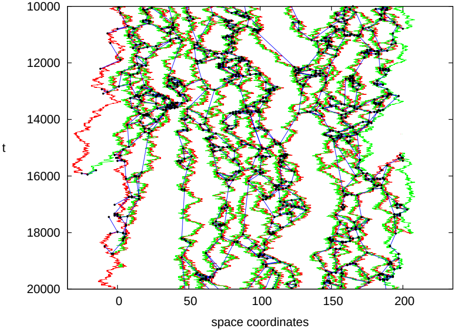


Analysis

The rates are the same by time reversal *symmetry*. How often do we have a branching/coalescing event?

To have just branching and coalescing points we use a **contraction** algorithm until there's no isolated point...

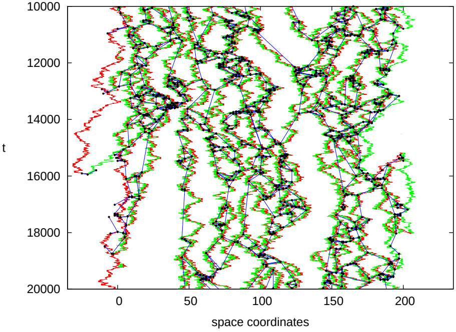




Analysis

The rates are the same by time reversal *symmetry*. How often do we have a branching/coalescing event?

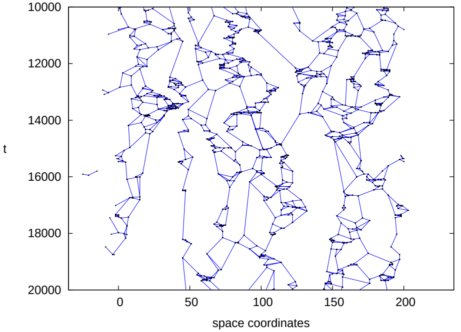
To have just branching and coalescing points we use a **contraction** algorithm until there's no isolated point...



Analysis

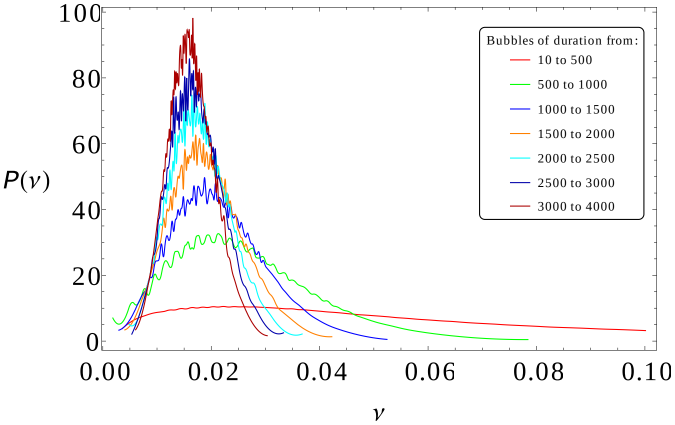
We end up with a brownian net with just branching and coalescing points.

How many events occur along the borders of a bubble? The frequency of branching/coalescing sould not depend on size of bubbles.



Probability distribution of frequency ν

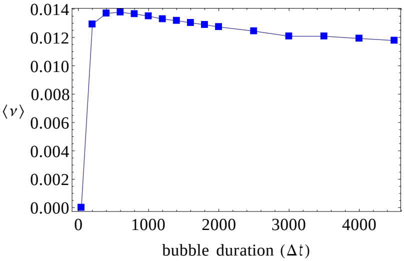
We can study the PDF of the frequency ν of branching and coalescing events for different bubbles' *sizes*.



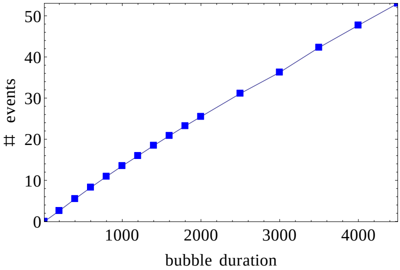
Average frequency

Are branching/coalescencing rates independent of bubble size?

Mean frequency $\bar{\nu}$:



Average number of events:



Perspectives

1. Check that the effective model from "brownian net" is realistic.
2. Convergence of the distribution of the event rates as statistics is increased
3. Determine average frequency $\bar{\nu}$?
4. How ν and D are related to c? Scaling limits?
5. What information do we have about the phase coexistence?
6. Low temperature limits for other KCM?
7. For a biased dynamics ($s < 0$ or $s > 0$), what can be relevant from this simple model?

Thank you for listening!

Bibliography

- Huang, Kerson. "Statistical mechanics." (1987)
- Chandler *et al*, Annu. Rev. Phys. Chem. 2010. **61**:191–217
- G. H. Fredrickson and H. C. Andersen Phys. Rev. Lett., 53(13):1244–1247, 1984
- T. Bodineau, V. Lecomte and C. Toninelli. J Stat Phys (2012) **147**:1–17
- J P Garrahan *et al* J. Phys. A: Math. Theor. 42 (2009) 075007
- S. Majumdar *et al* J Stat. Phys. **119**.3-4 (2005): 777-826.
- Majumdar, Satya N. arXiv preprint cond-mat/0510064 (2005).
- D. Chandler *et al.* Phys Rev X 1, 021013 (2011)

Order parameter

Activity

$$K = \Delta t \sum_{t=0}^{t_{\text{obs}}} \sum_{i=1}^{L} (r_i(t+\Delta t) - r_i(t))^2$$

where L is the total number of particles considered and t_{obs} is the amount of time the systems is observed.
The mean *activity* is

$$\langle K \rangle = L t_{\text{obs}} \langle (r_1(t+\Delta t) - r_1(t))^2 \rangle = 2dLt_{\text{obs}} D \Delta t$$

Tests

For an **unconstrained model**, the probability of a configuration $\vec{n} = (n_1, n_2, \ldots, n_L)$ is $P_{eq}^{unc}(\vec{n}) = c^n(1-c)^{L-n}$, therefore the average value of a site is

$$\boxed{\frac{1}{L}\left\langle \sum_i n_i \right\rangle_{eq}^{unc} = c}.$$

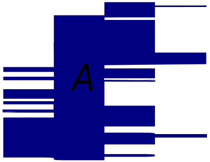
For a **constrained model** where $\sum_i^L n_i > 0$, the probability has a normalization factor Z $P_{eq}(\vec{n}) = \frac{c^n(1-c)^{L-n}}{Z}$ which is found to be $Z = 1-(1-c)^L$. The average value of a site is

$$\boxed{\langle n_j \rangle_{eq} = \frac{c}{1-(1-c)^L}}.$$

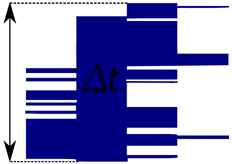
We compare this value with the one obtained numerically. The bigger the lattice, the more accurate the numerical value is.

Temporal Perimeter

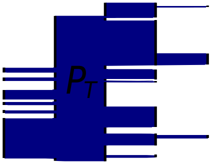
Area



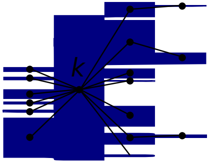
Temporal extension



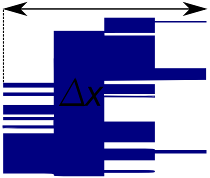
Temporal perimeter



Number of Nodes

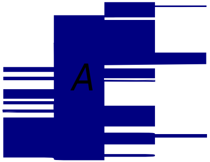


Spatial extension

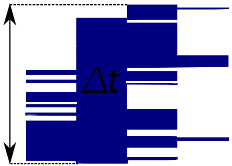


Spatial Perimeter

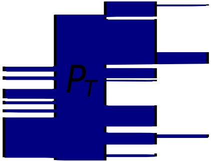
Area



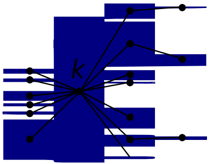
Temporal extension



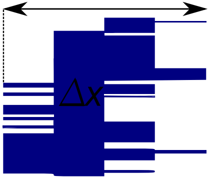
Temporal perimeter



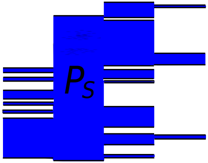
Number of Nodes



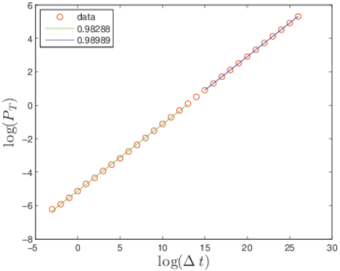
Spatial extension



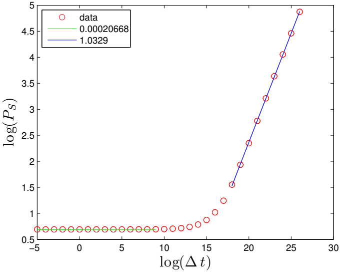
Spatial perimeter



Perimeter geometry



(g)



(h)

$P_T \sim \Delta t$ for all of the bubbles and $P_S \sim \Delta t$ for large bubbles.