Deposition, diffusion, and nucleation on an interval

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Joint work with Andrew Wade (Durham University)

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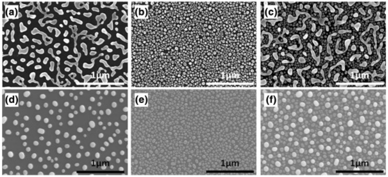
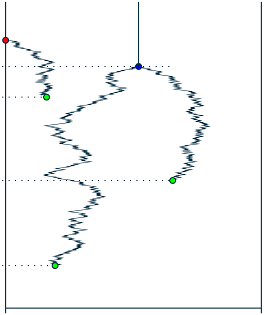
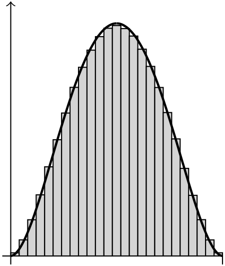
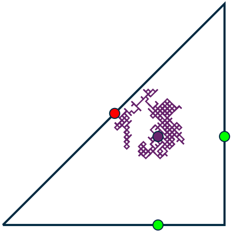
Image gallery









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Motivation: Nanoscale growth of ultrathin films

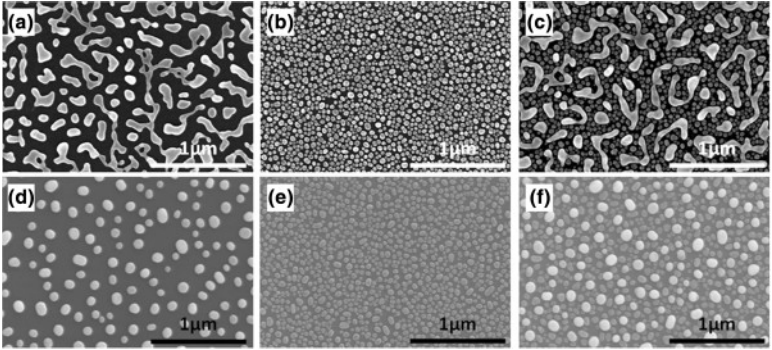

Image credit: Tan et al., Nanoscale Research Letters 2014, **9**:181.

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Model definition

- System starts with a single interval $[0, 1]$ that has two islands at endpoints 0 and 1
- Particles are deposited at rate $\lambda > 0$ onto $[0, 1]$ (i.e., according to a Poisson process on $\mathbb{R}_+ \times [0, 1]$ with intensity λ)
- Upon arrival, each particle performs Brownian motion (independently) until either:
  1. a moving particle hits an existing island and is absorbed; or
  2. two moving particles meet and "nucleate", forming a new island
- In either case, those particles stop moving (in effect, removed from the system)

Note: nucleation splits an existing interval into two new ones which then evolve independently.

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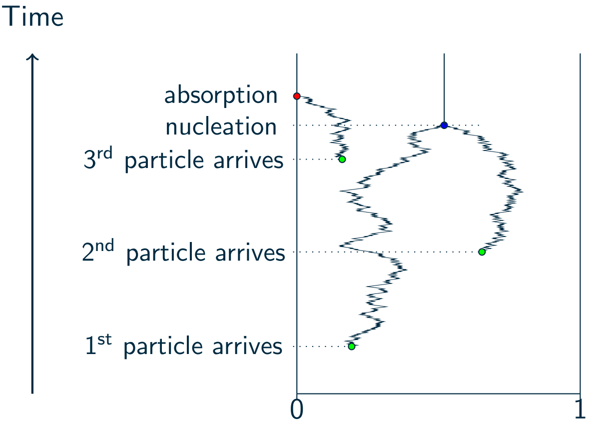
Model definition: in pictures



Induced interval-splitting process

This yields a well-defined Markov process $(\mathcal{Y}_t)_{t \geq 0}$ for all time. (Enough for $\mathcal{Y}$ to include positions of all islands and all active particles.)

We focus attention on the interval-splitting process induced by the nucleations.

After n nucleations, there are $n+1$ interval lengths $\mathcal{L}_n = (L_{n,0}, L_{n,1}, \dots, L_{n,n})$.
Note: $L_{n,j} > 0$ and $\sum_j L_{n,j} = 1$ for all $n \geq 0$.

The process $\mathcal{L} = (\mathcal{L}_0, \mathcal{L}_1, \dots)$ is not itself Markovian, since it depends also on positions of active particles.

Main result: convergence to a Markovian interval-splitting process in the sparse deposition limit ($\lambda \to 0$).

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Markovian interval-splitting process

Specified by two parameters r and Φ:

- the function $r : [0,1] \to \mathbb{R}_+$ controls which interval is selected to be split
- the probability measure Φ on $[0,1]$ (with $\Phi(\{0\}) = 0$ and $\Phi(\{1\}) = 0$) controls where along its length the selected interval is to be split

Given current state $(\ell_1, \ldots, \ell_k)$ of interval lengths (where $\ell_i > 0$ and $\sum_i \ell_i = 1$) update rule is:

1. Select interval j to be split, with probability proportional to $r(\ell_j)$
2. Length ℓ_j is replaced by the two lengths $x\ell_j$ and $(1-x)\ell_j$ where $x \in [0,1]$ is distributed according to Φ

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Convergence to Markovian interval-splitting process

Theorem 1 (GW, 2020+)

As $\lambda \to 0$, the process $\mathcal{L}$ converges* to the Markovian interval-splitting process with parameters r_0 and Φ_0.

- $r_0(\ell) := \ell^4$
- Φ_0 is the probability measure on $[0,1]$ with density proportional to ψ defined as

$$\psi(z) := \frac{24}{\pi^4} \sum_{n \text{ odd}} a_n \sin(n\pi z); \qquad a_n := \frac{4}{n^4} \tanh\left(\frac{n\pi}{2}\right) - \frac{\pi}{n^3}$$

*TV-convergence of finite dimensional distributions

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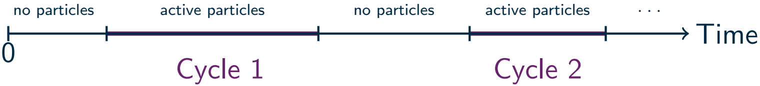
Proof ideas

- Exploit regenerative structure:



- No nucleation in a cycle $\implies$ system in same state as end of previous cycle
- For very small λ, probability of nucleation in the next cycle dominated by probability that 2 particles arrive in the same interval and meet, before either is absorbed.
- Parameter $r_0(\ell) = \ell^4$ arises from a scaling property relating the process on $[0, \ell]$ with rate λ to the process on $[0, 1]$ with rate $\ell^3\lambda$.

Brownian motion exiting a triangle

For $B \subseteq [0,1]$, define $\Psi(B) = \int_B \psi(z)\mathrm{d}z$. Recall: $\Phi_0(B) = \frac{\Psi(B)}{\Psi([0,1])}$.

The measure Ψ arises from an exit problem for Brownian motion in a right-angled triangle:

Lemma

$$\Psi(B) = \int_0^1 \mathrm{d}z \int_0^1 \mathrm{d}y \int_0^1 \mathrm{d}x \int_0^\infty q_t(x,y) H(\{y,z\}; B)\mathrm{d}t$$

- $q_t(x,y)$ — the density (at position y and time t) of absorbed Brownian motion on $[0,1]$ started at x at time 0.
- $H(\{u,v\}; B)$ — (for $u > v$) the probability that 2-dim Brownian motion started at (u,v) exits the triangle through $\widetilde{B} := \{(w,w) : w \in B\}$.

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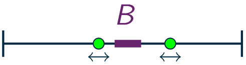
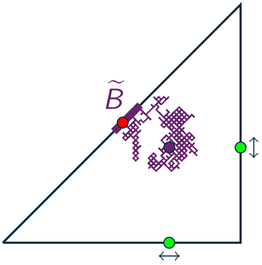
Brownian motion exiting a triangle

Lemma

$$\Psi(B) = \int_0^1 \mathrm{d}z \int_0^1 \mathrm{d}y \int_0^1 \mathrm{d}x \int_0^\infty q_t(x,y) H(\{y,z\}; B) \mathrm{d}t$$

- x — arrival position of 1st particle
- t — time between arrivals of 1st and 2nd particles
- y — position of 1st particle at time t
- z — arrival position of 2nd particle





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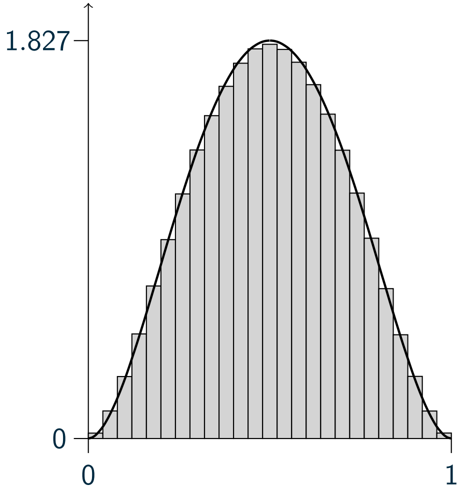
Density of Φ_0

$$\psi(z) := \frac{24}{\pi^4} \sum_{n \text{ odd}} a_n \sin(n\pi z); \qquad a_n := \frac{4}{n^4} \tanh\left(\frac{n\pi}{2}\right) - \frac{\pi}{n^3}$$



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Convergence of empirical gap size distribution

For fixed λ, we have almost sure convergence of the (normalised) empirical gap size distribution:

Definition

$$\mathcal{E}_n(x) := \frac{1}{n+1} \sum_{j=1}^{n+1} \mathbf{1}\left\{ L_{n,j} \leq \frac{x}{n+1} \right\}$$

Theorem 2 (GW, 2020+)

Let $\lambda \in (0, \infty)$. There is a continuous probability density g_0 on $\mathbb{R}_+$ (described in terms of r_0 and Φ_0) such that, for all $x \in \mathbb{R}_+$,

$$\mathcal{E}_n(x) \to \int_0^x g_0(y) \mathrm{d}y, \text{ a.s., as } n \to \infty.$$

Moreover, there exist positive constants c_0, c_∞ and θ such that

$$g_0(x) \sim c_0 x^2, \text{as } x \to 0, \text{ and } g_0(x) \sim c_\infty x^{-2} \exp\left(-\theta x^4\right), \text{as } x \to \infty.$$

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Slides at `http://community.dur.ac.uk/nicholas.georgiou/`

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Thanks for watching!