Can Monte Carlo methods be used to simulate active-matter systems?

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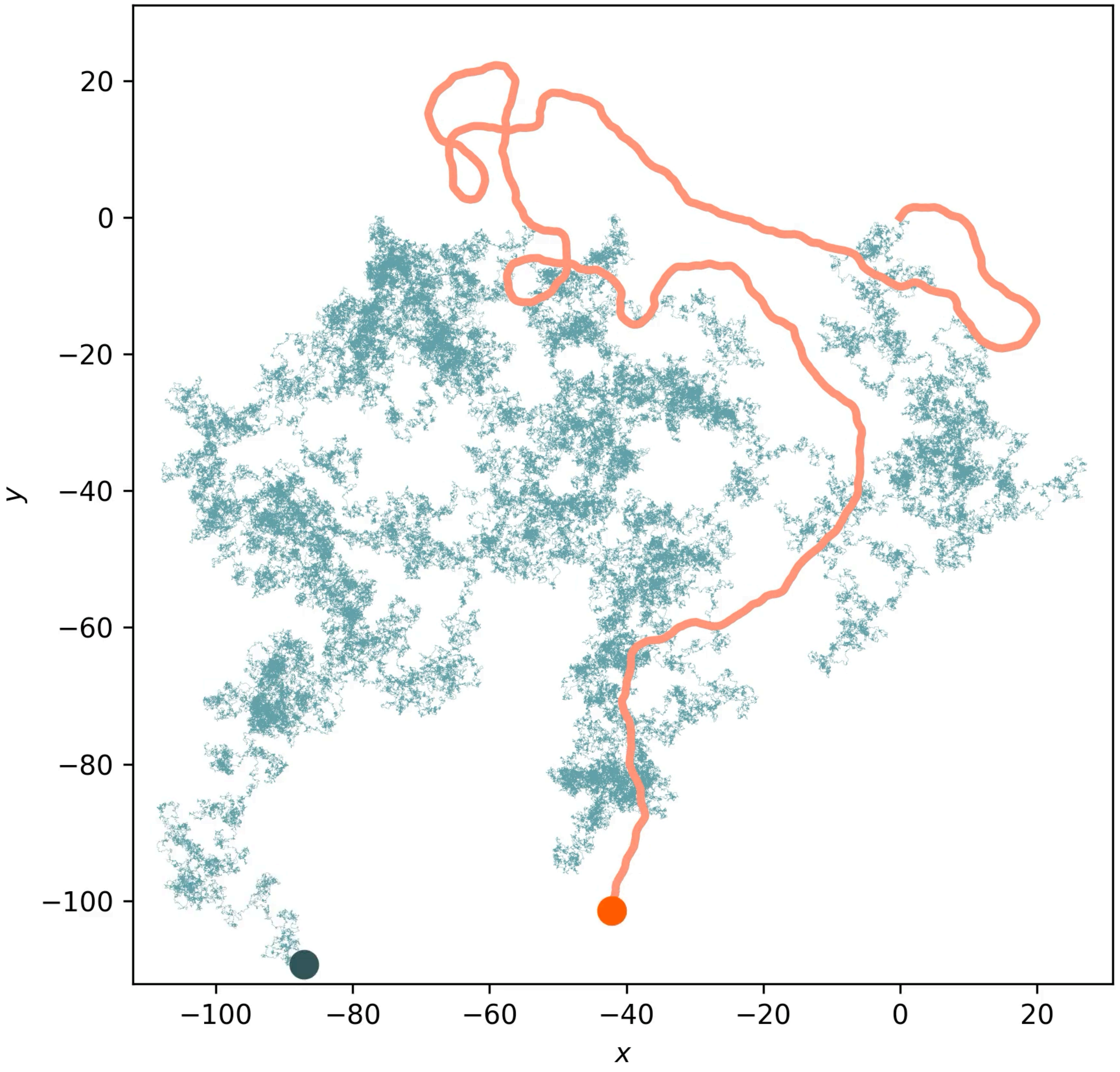
(3) Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.

What is Active Matter?



Brownian motion

$$\mathbf{v}(t) := \frac{d\mathbf{r}(t)}{dt} = \sqrt{2D}\,\boldsymbol{\eta}(t)$$

$$\langle \eta_x(t)\eta_y(t') \rangle = \delta_{x,y}\delta(t-t')$$

Detailed Balance

Active Brownian particle

NO Detailed Balance

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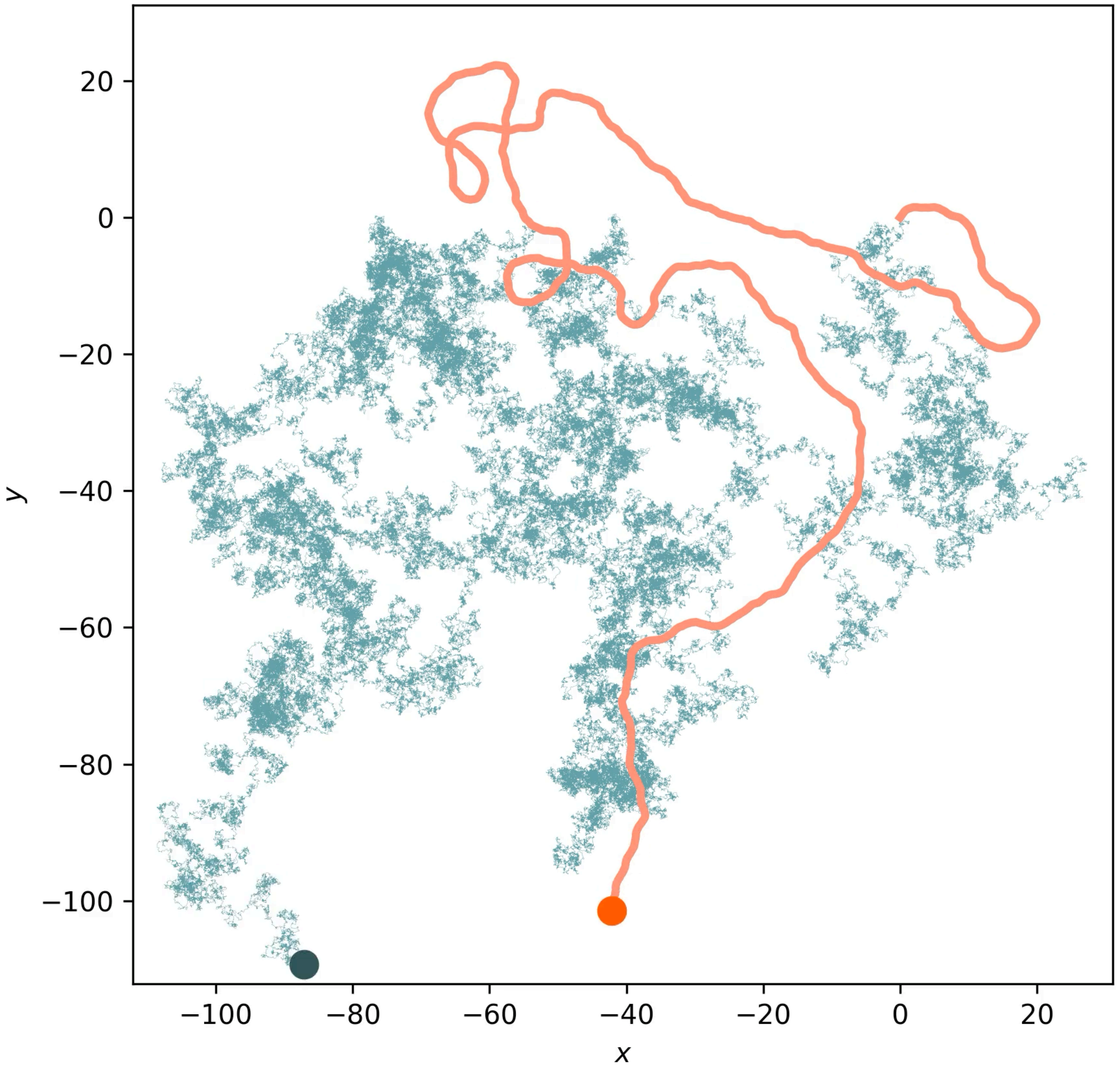

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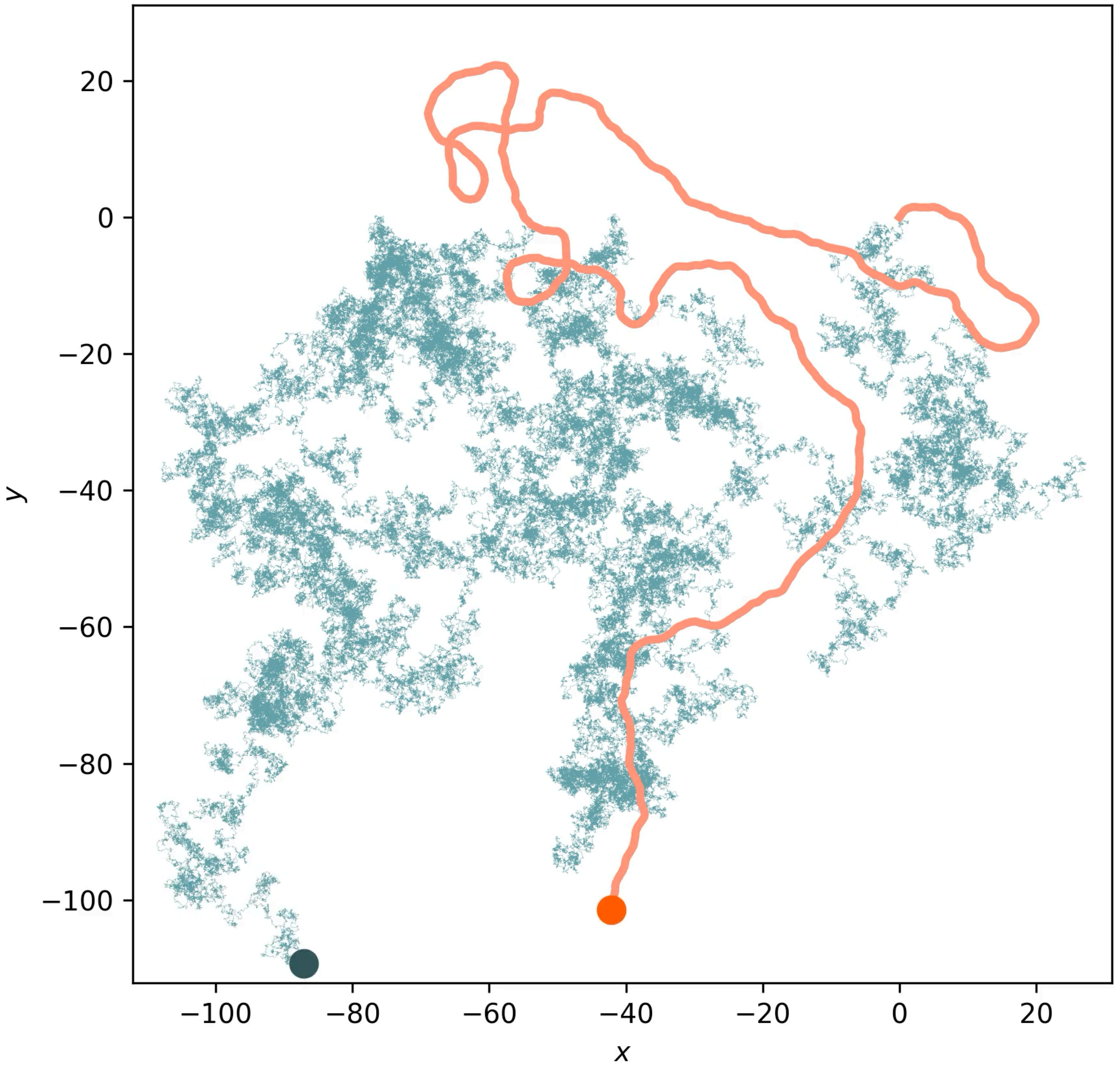

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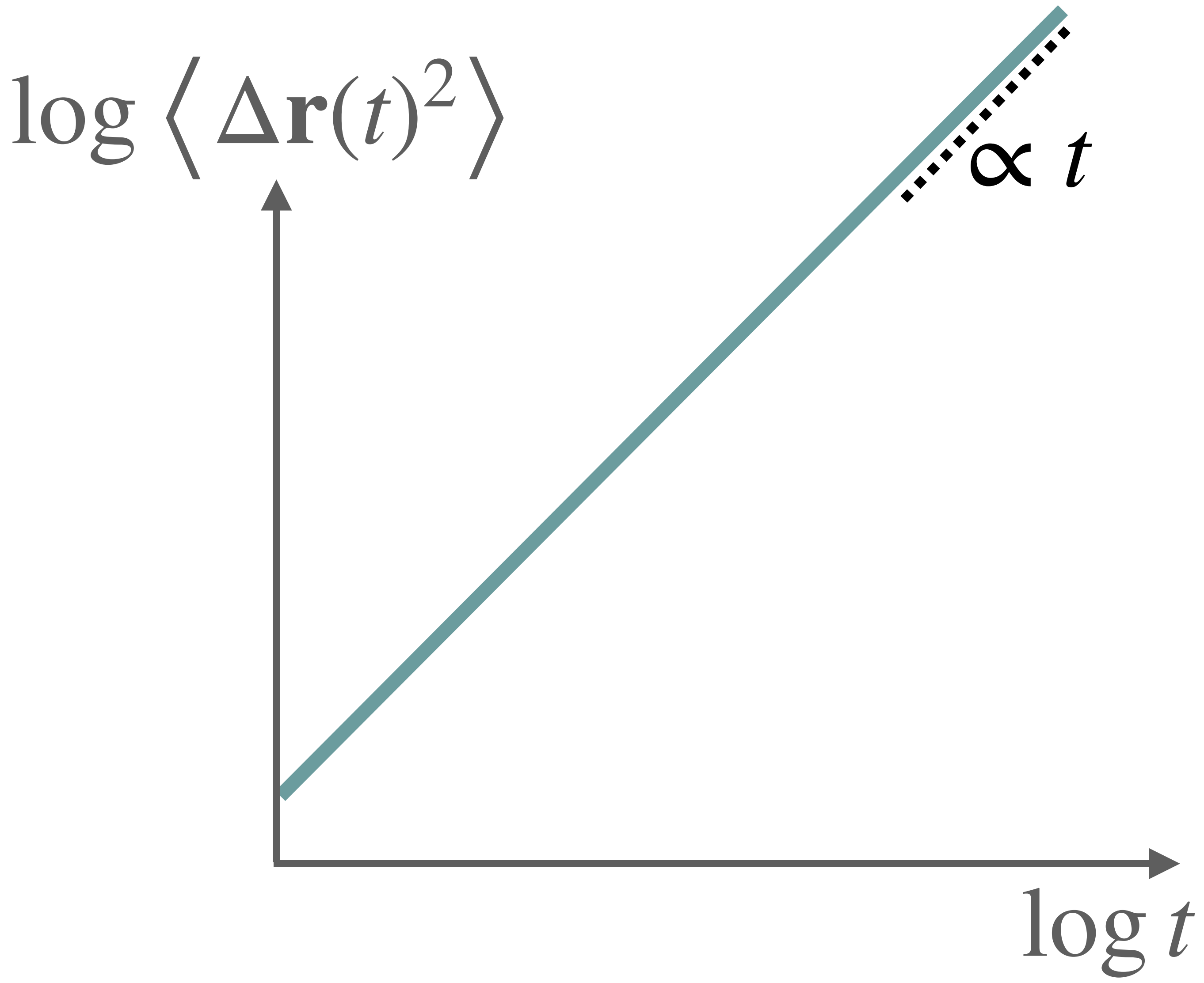

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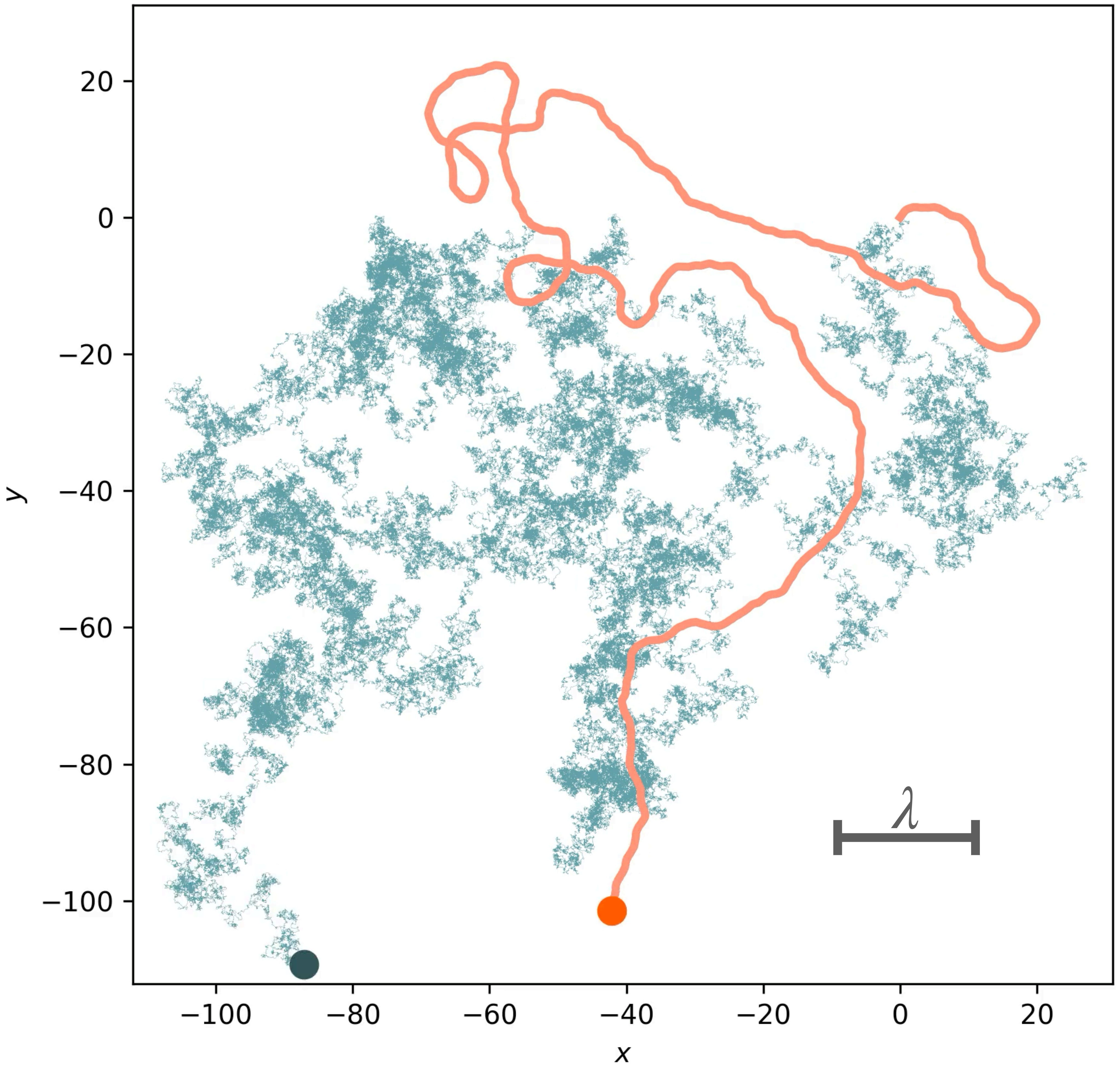

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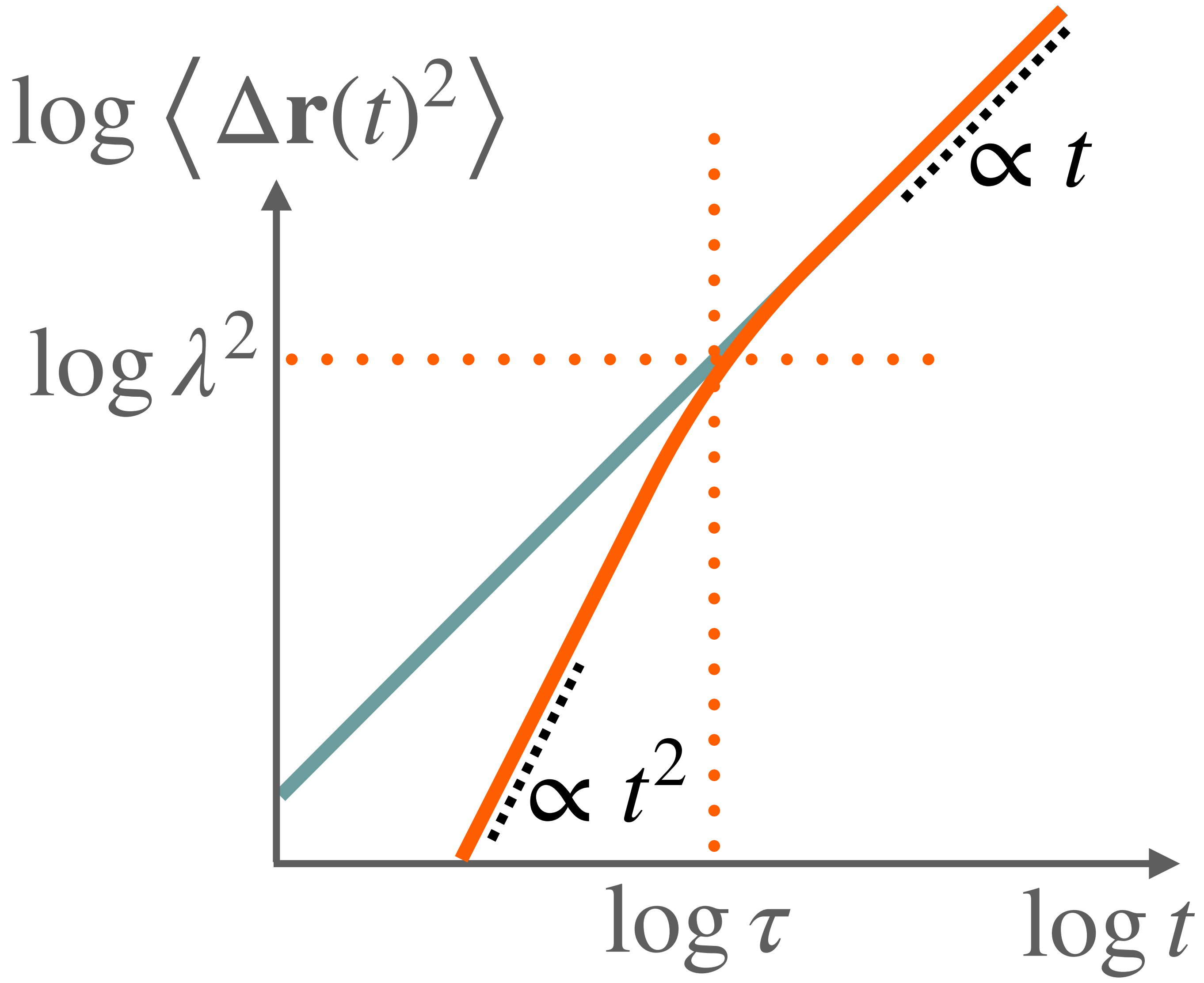

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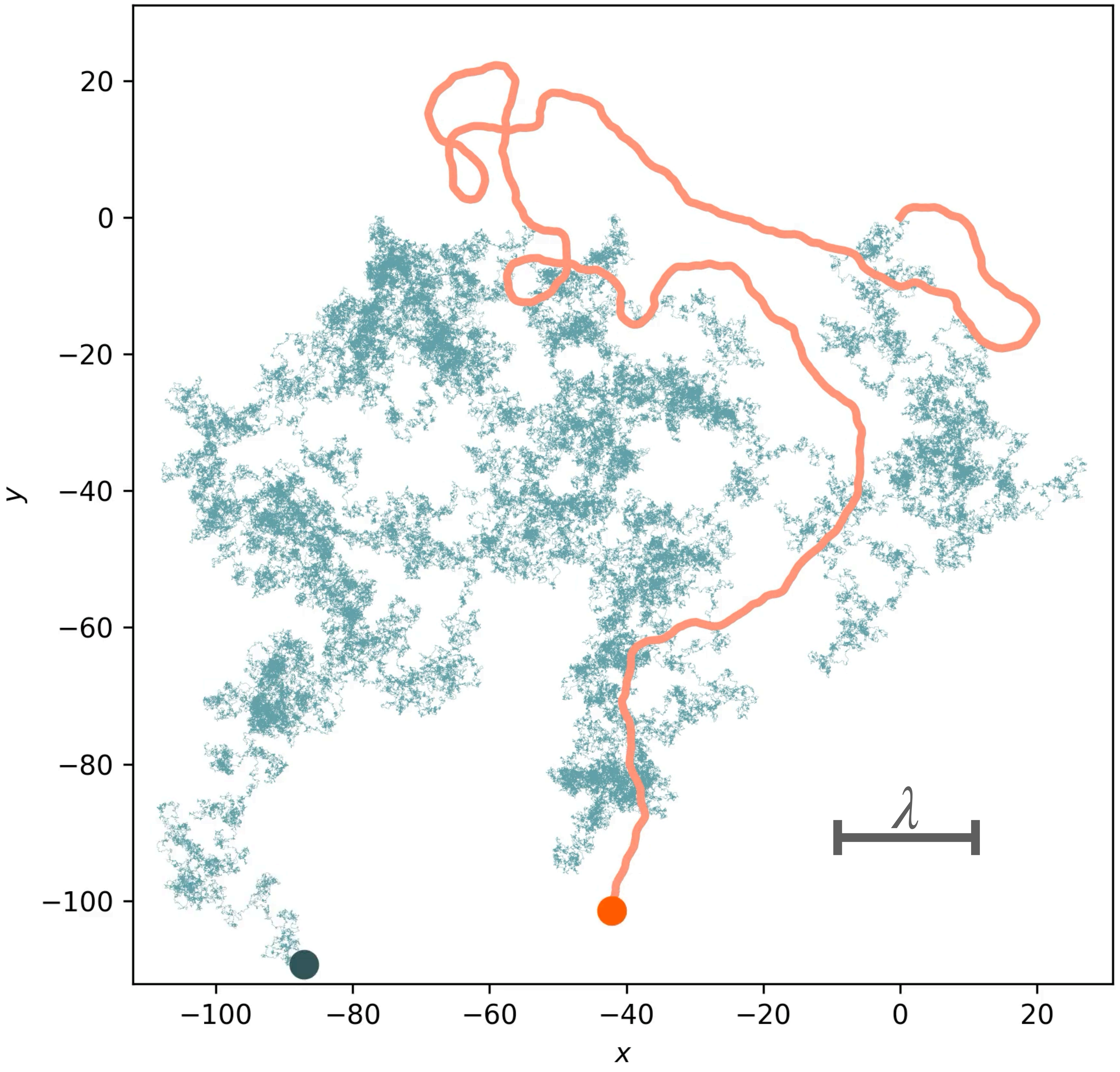

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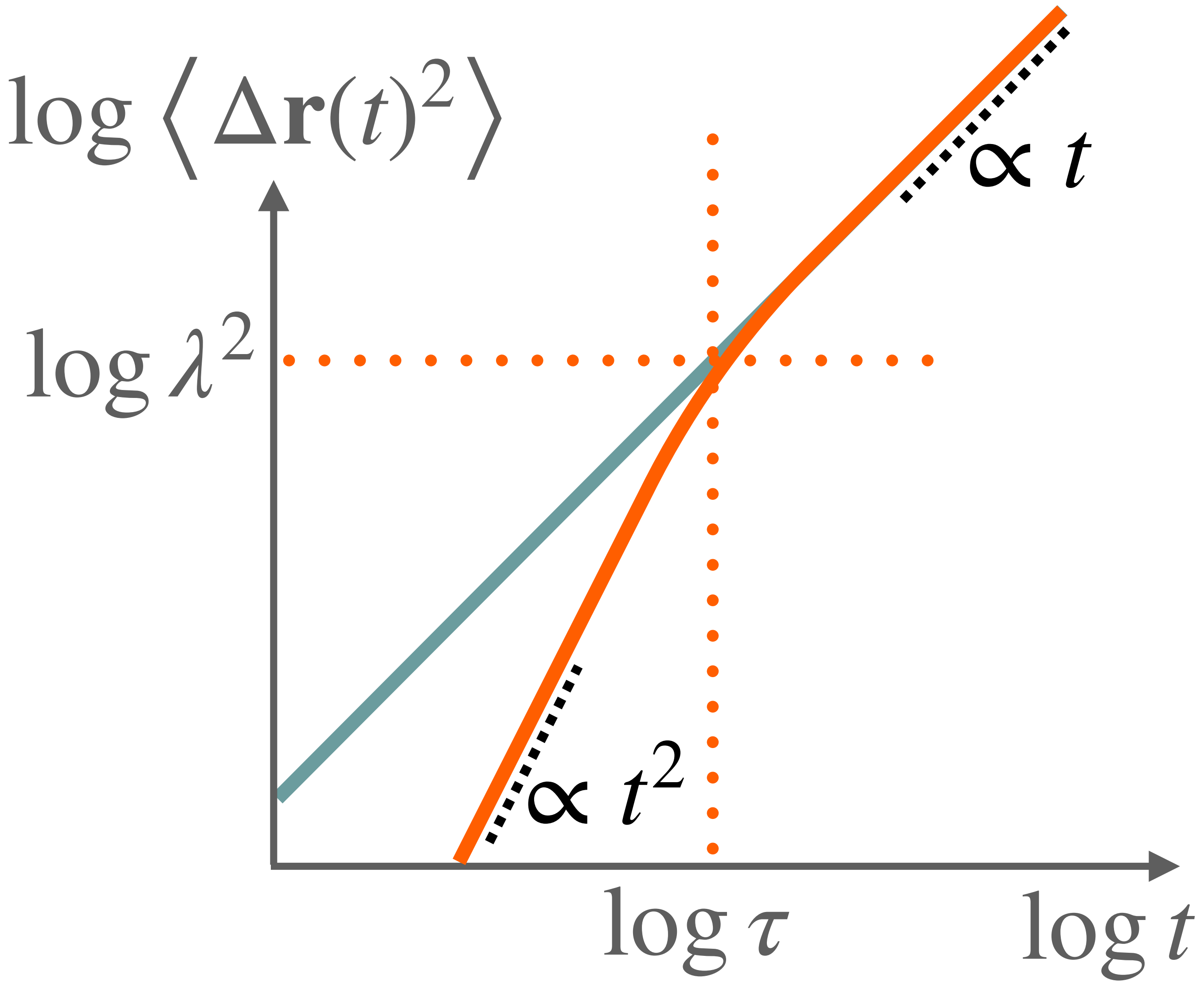

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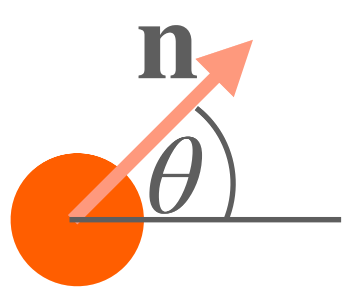

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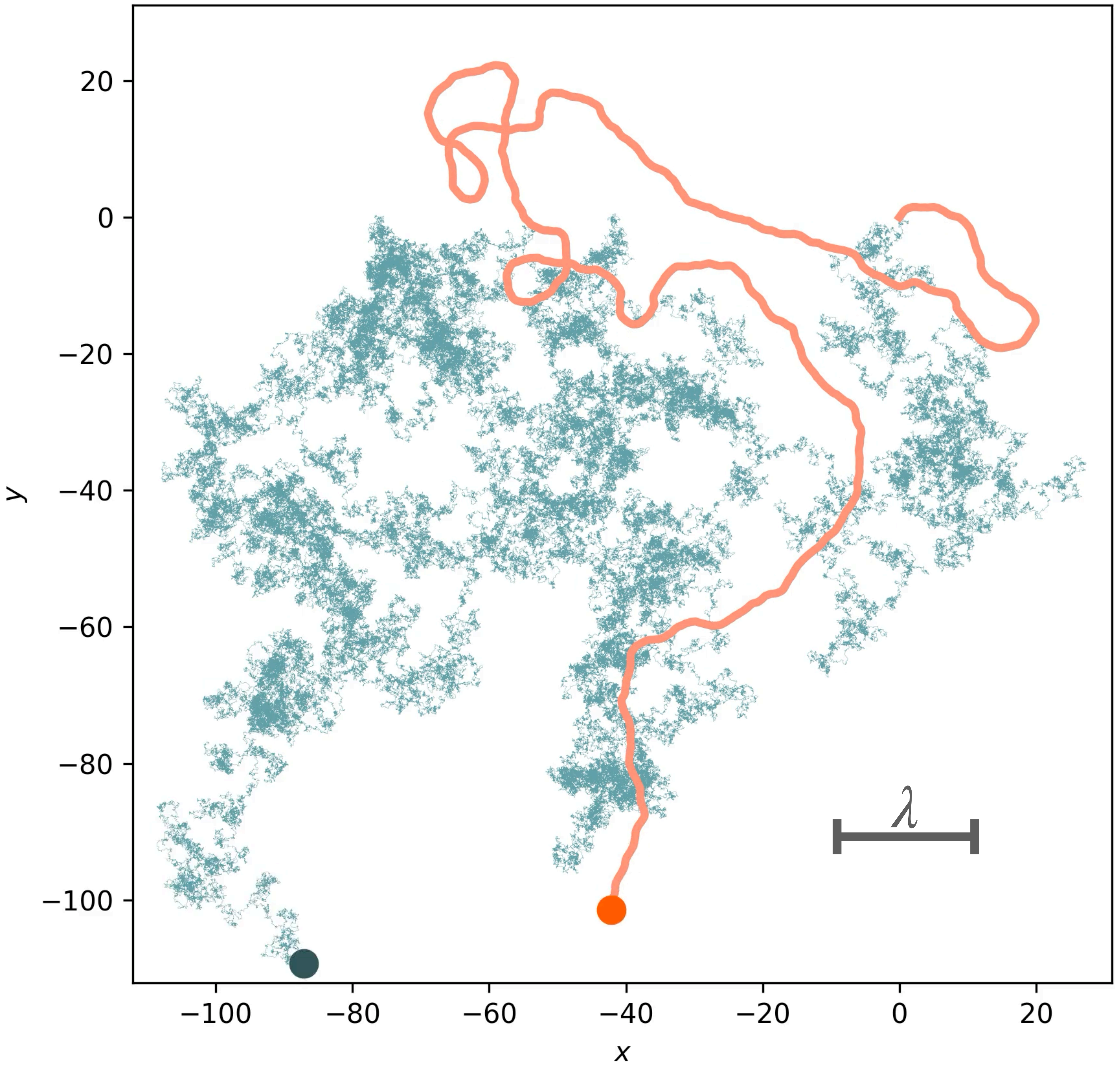

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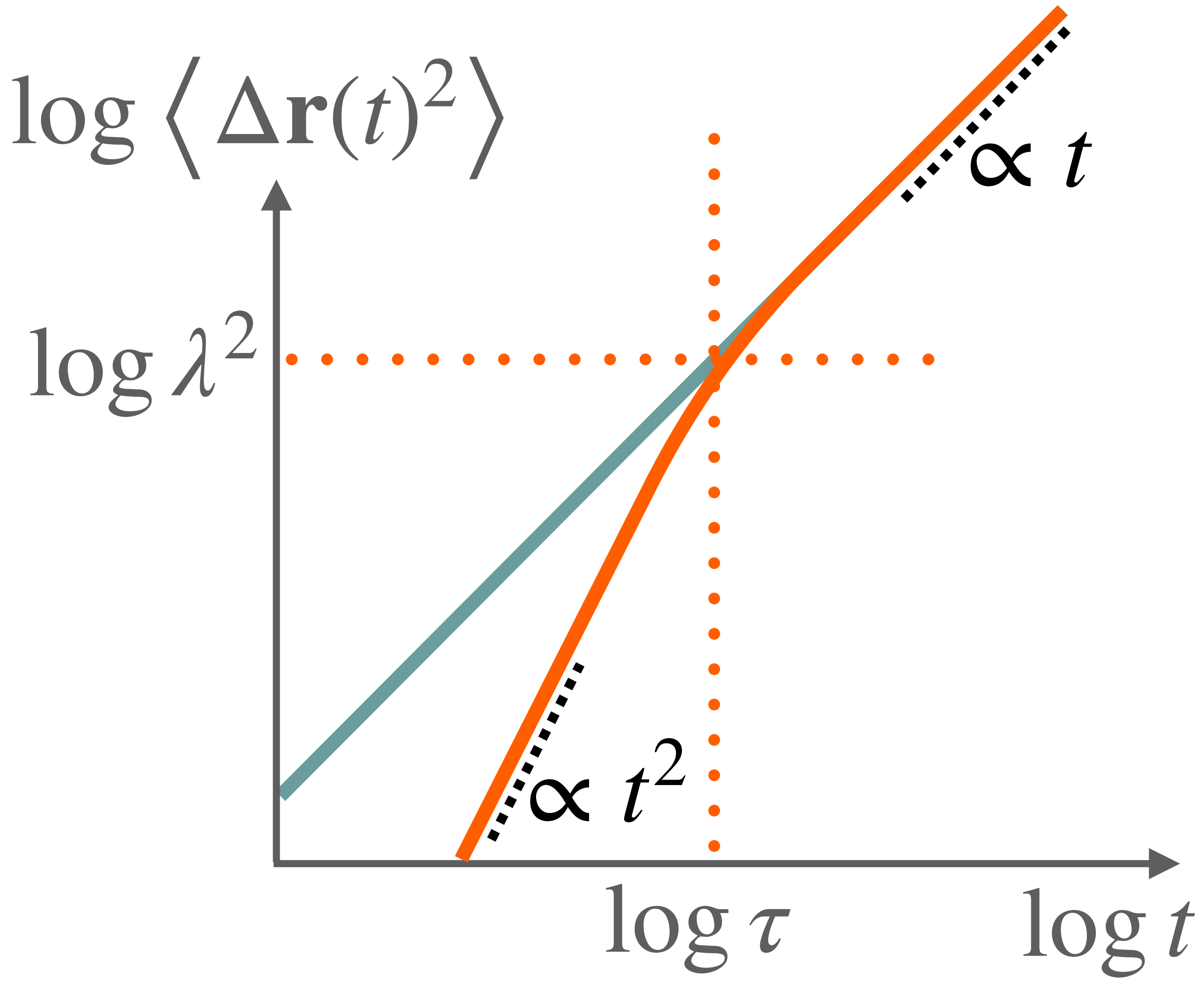

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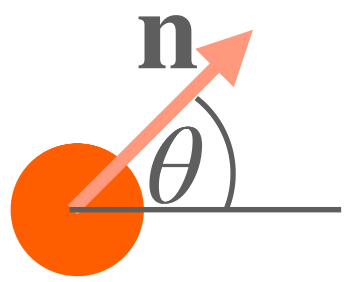

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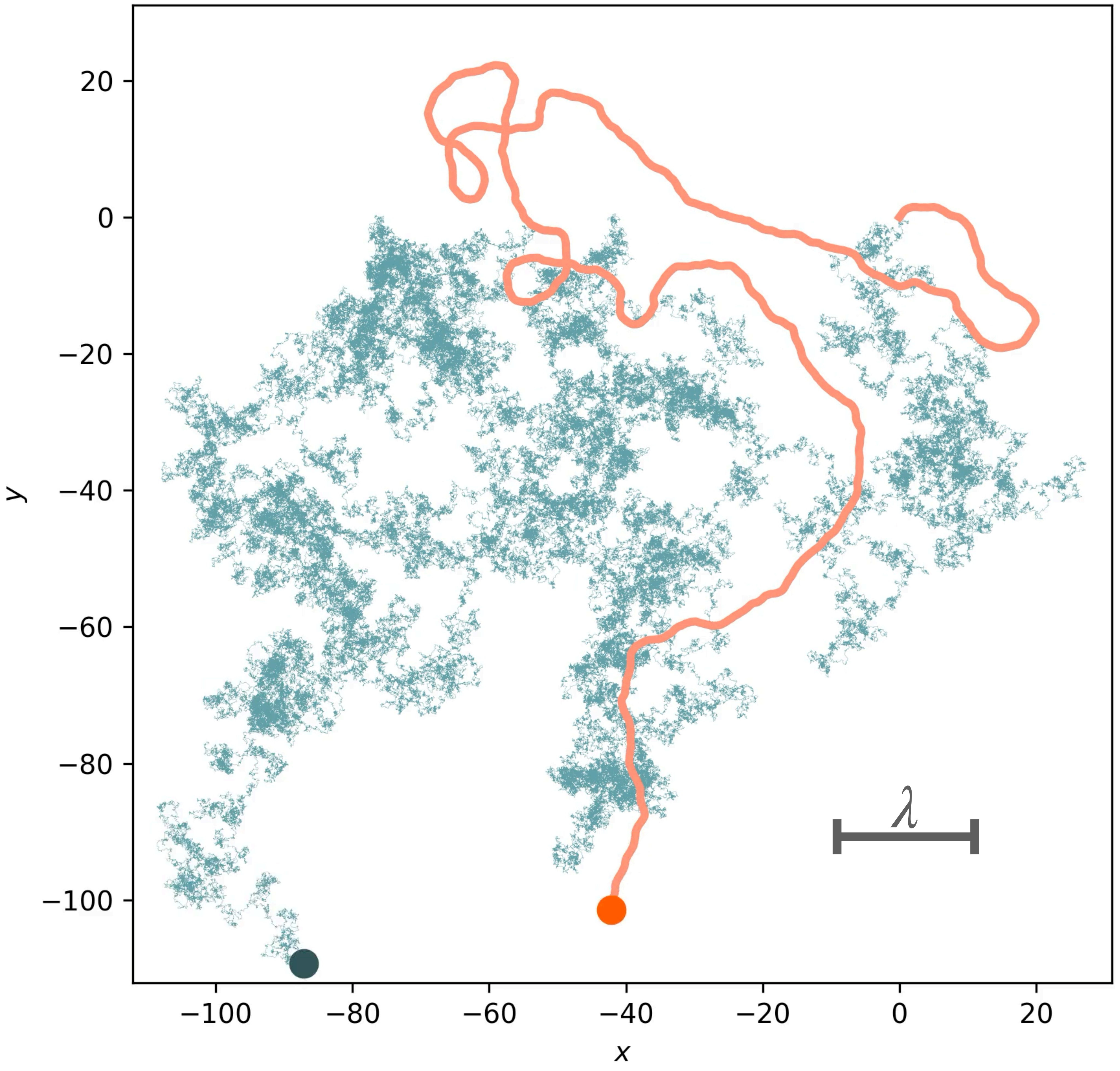

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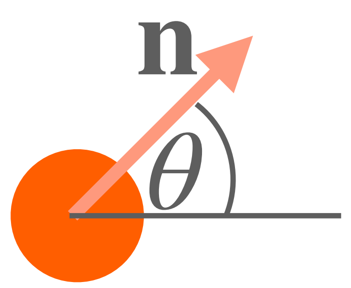

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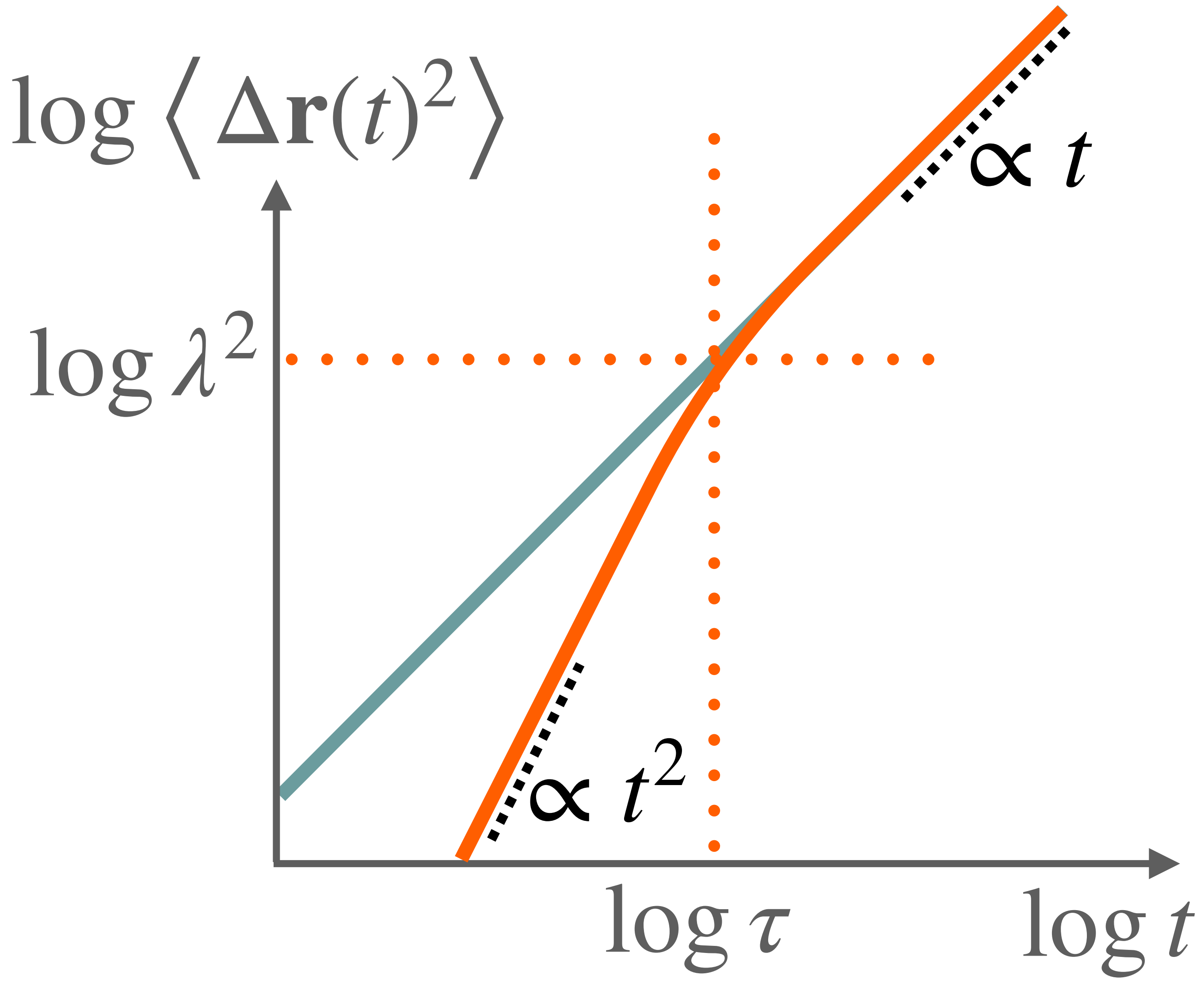

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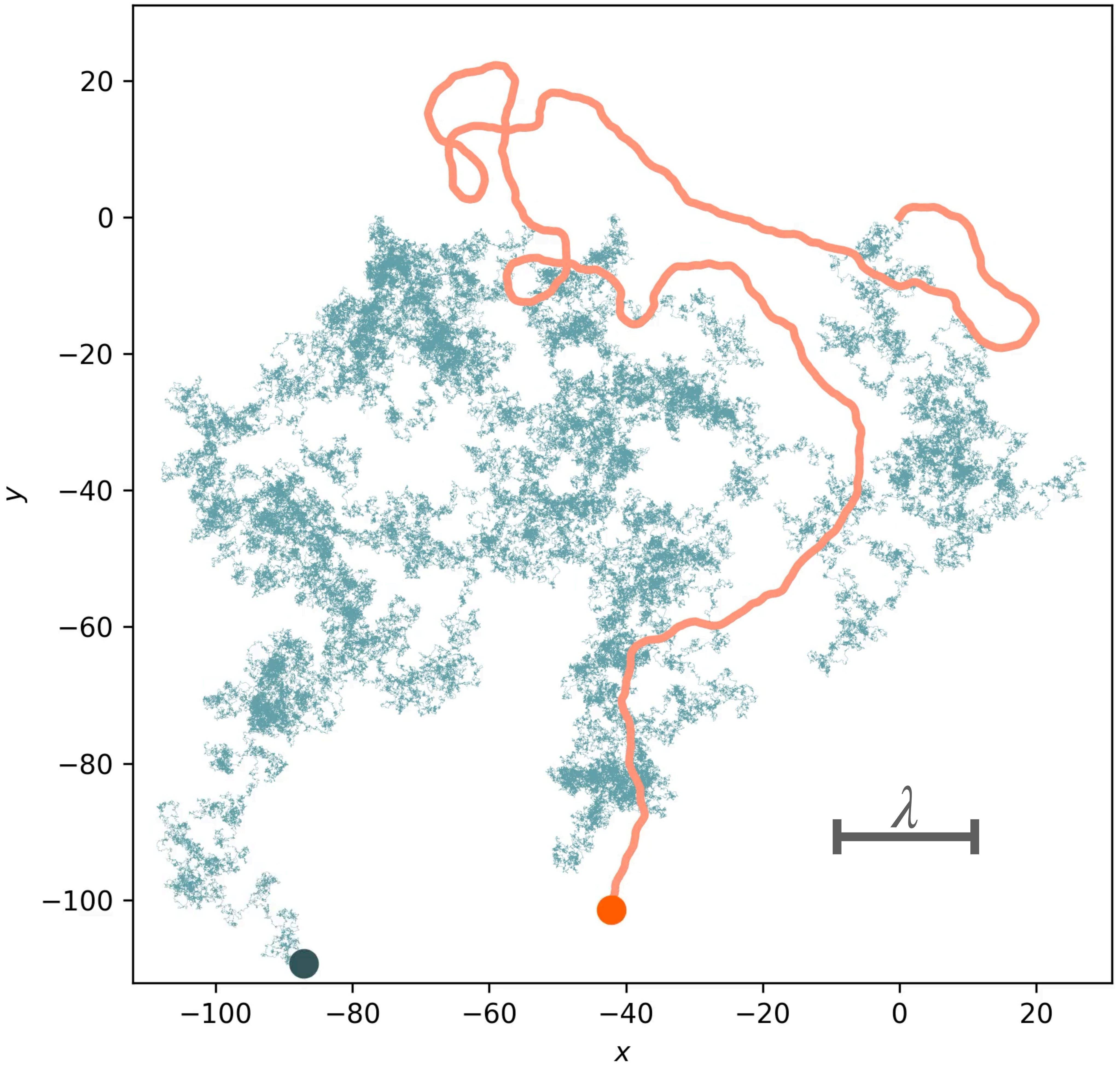

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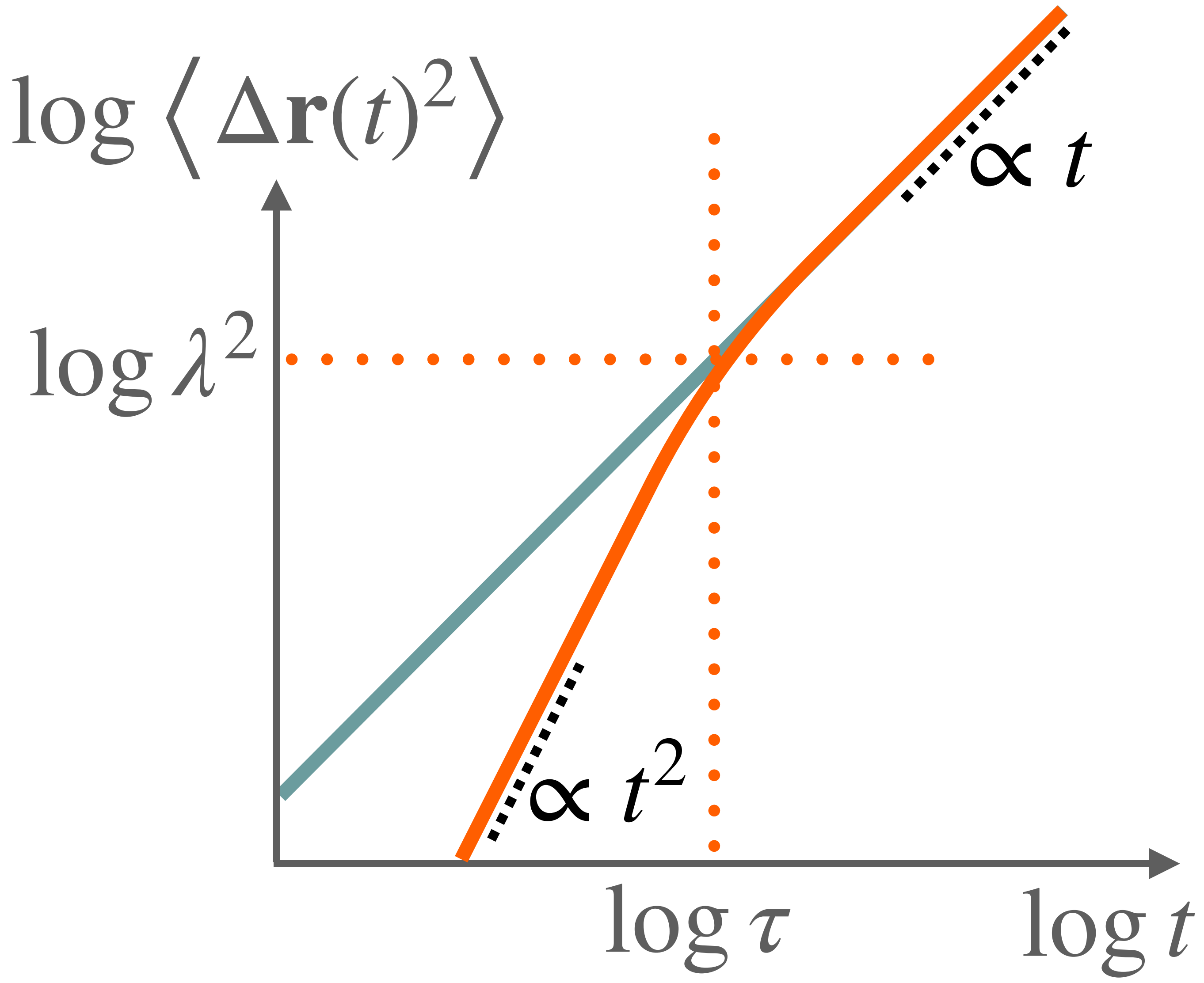

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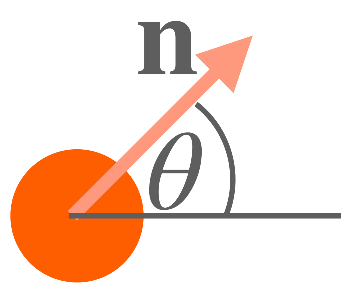

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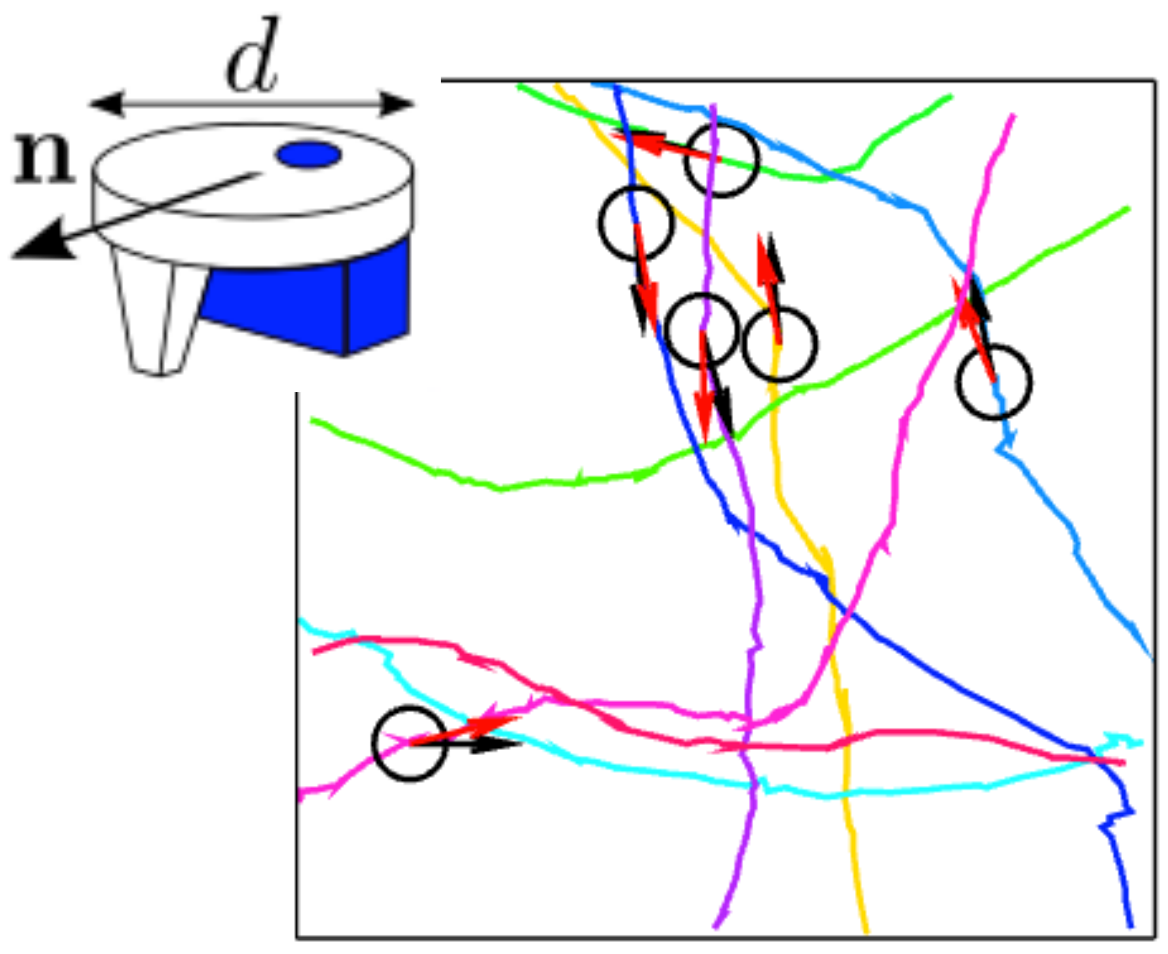
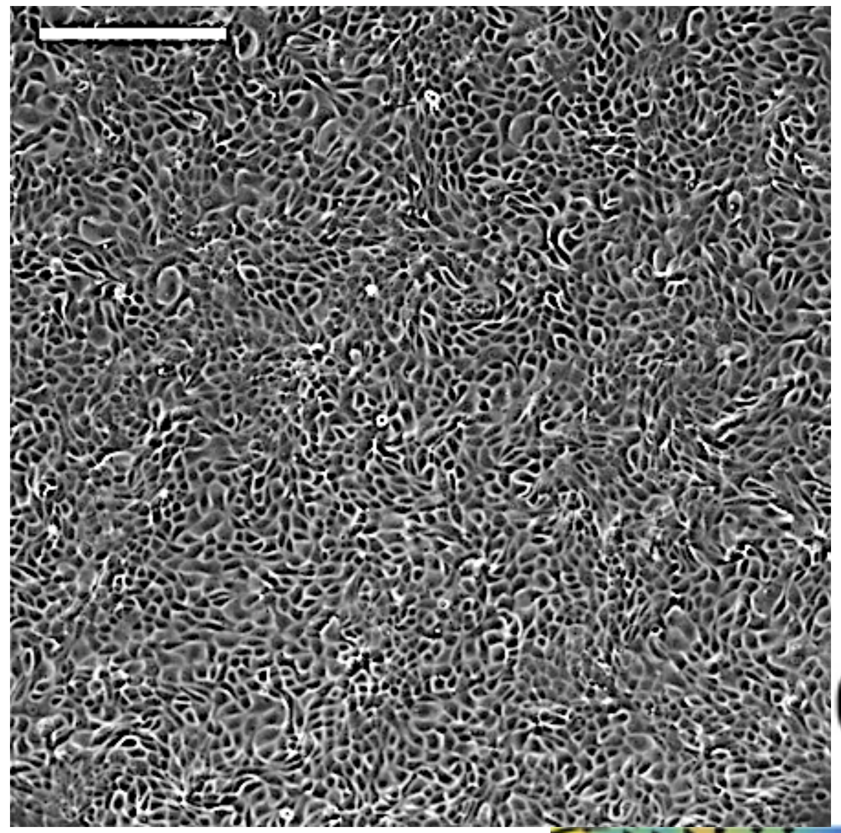
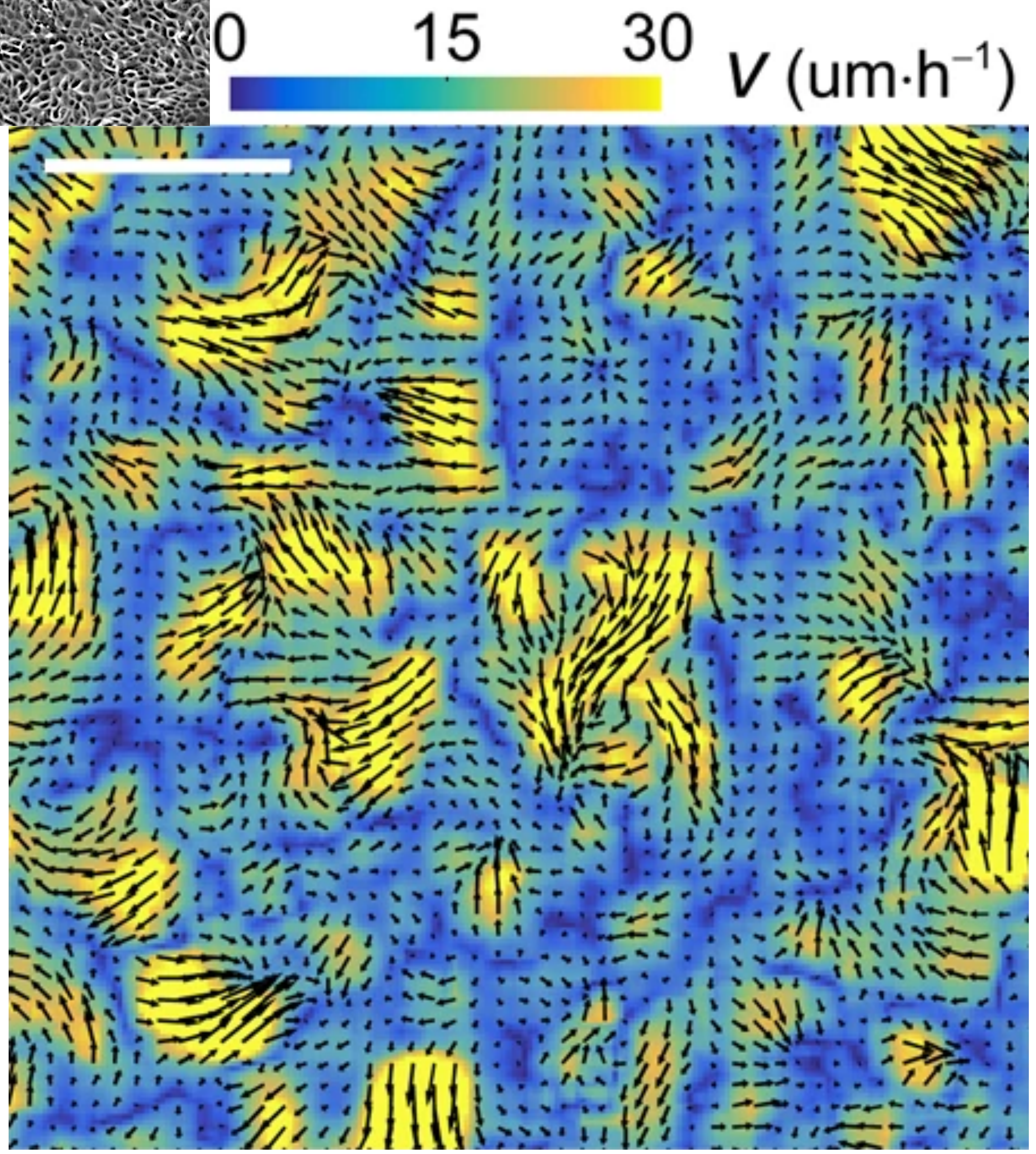


J. Deseigne, O. Dauchot, H. Chaté
PRL 105, 098001 (2010).

Collective phenomena in active matter



Complex chaotic flows
in monolayers of cells



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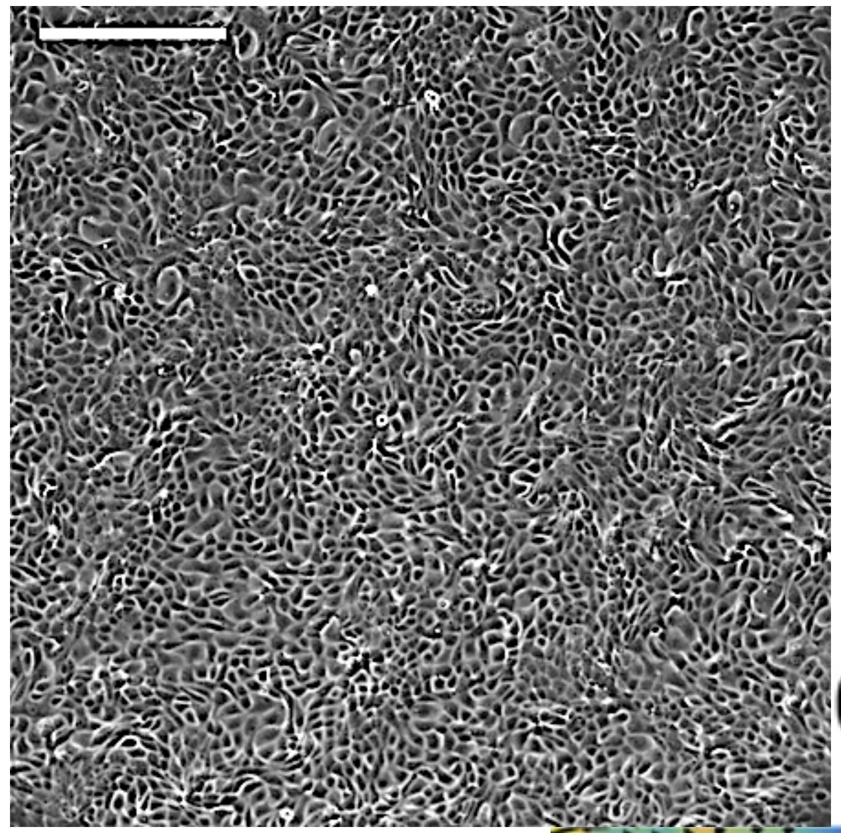

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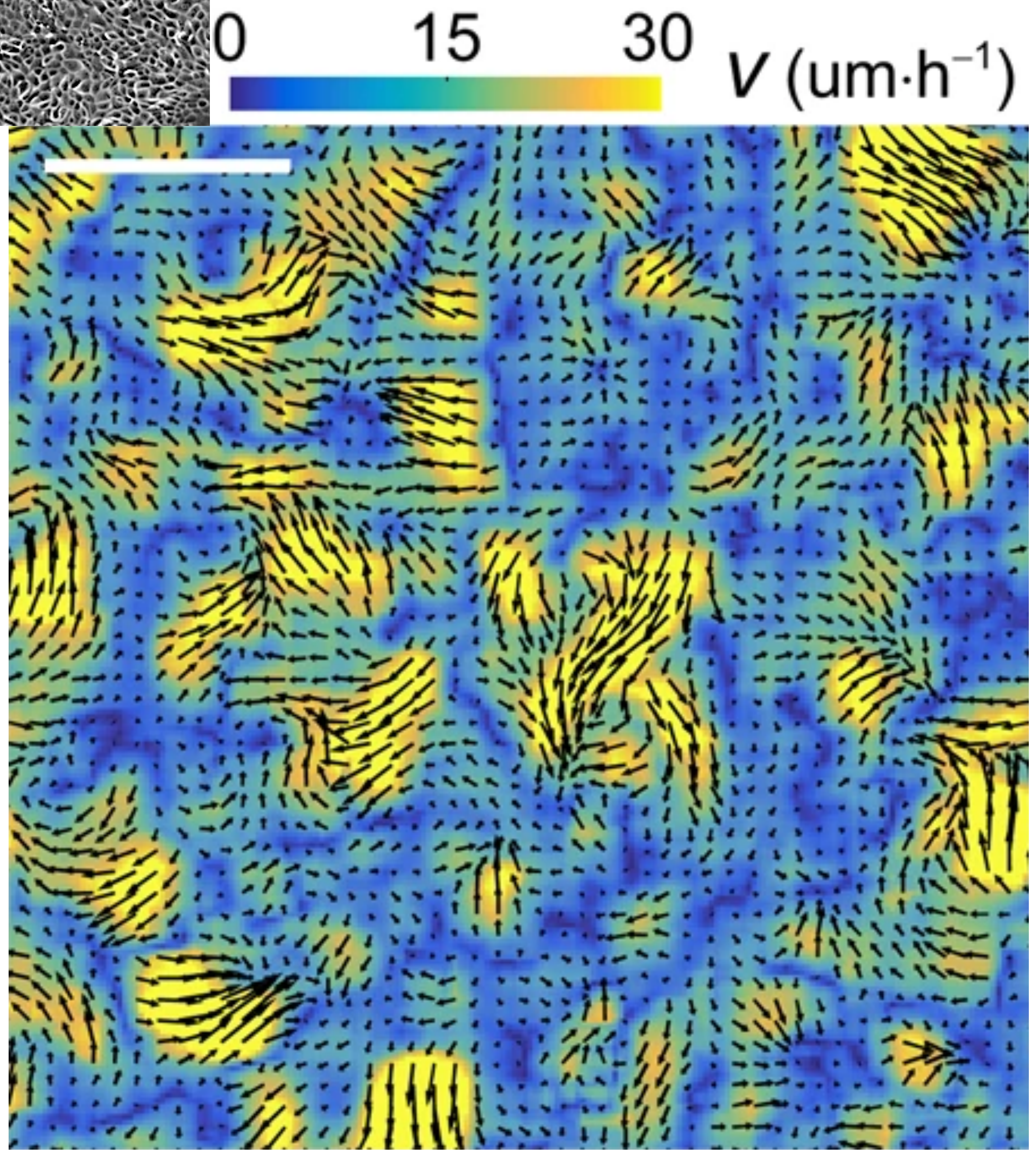

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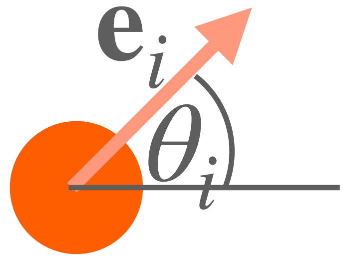

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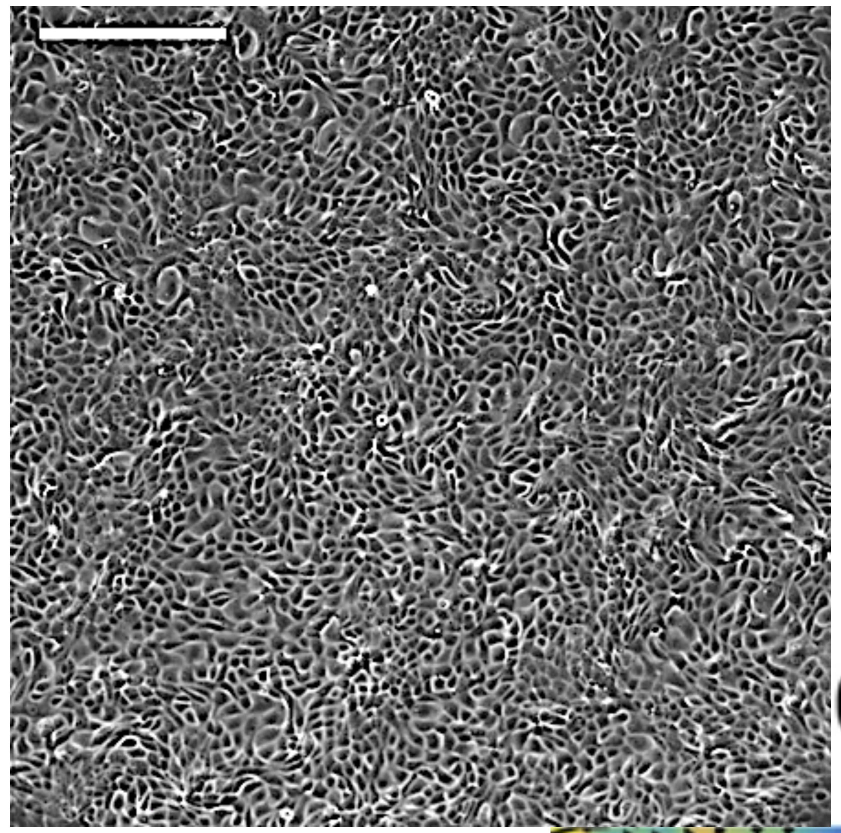

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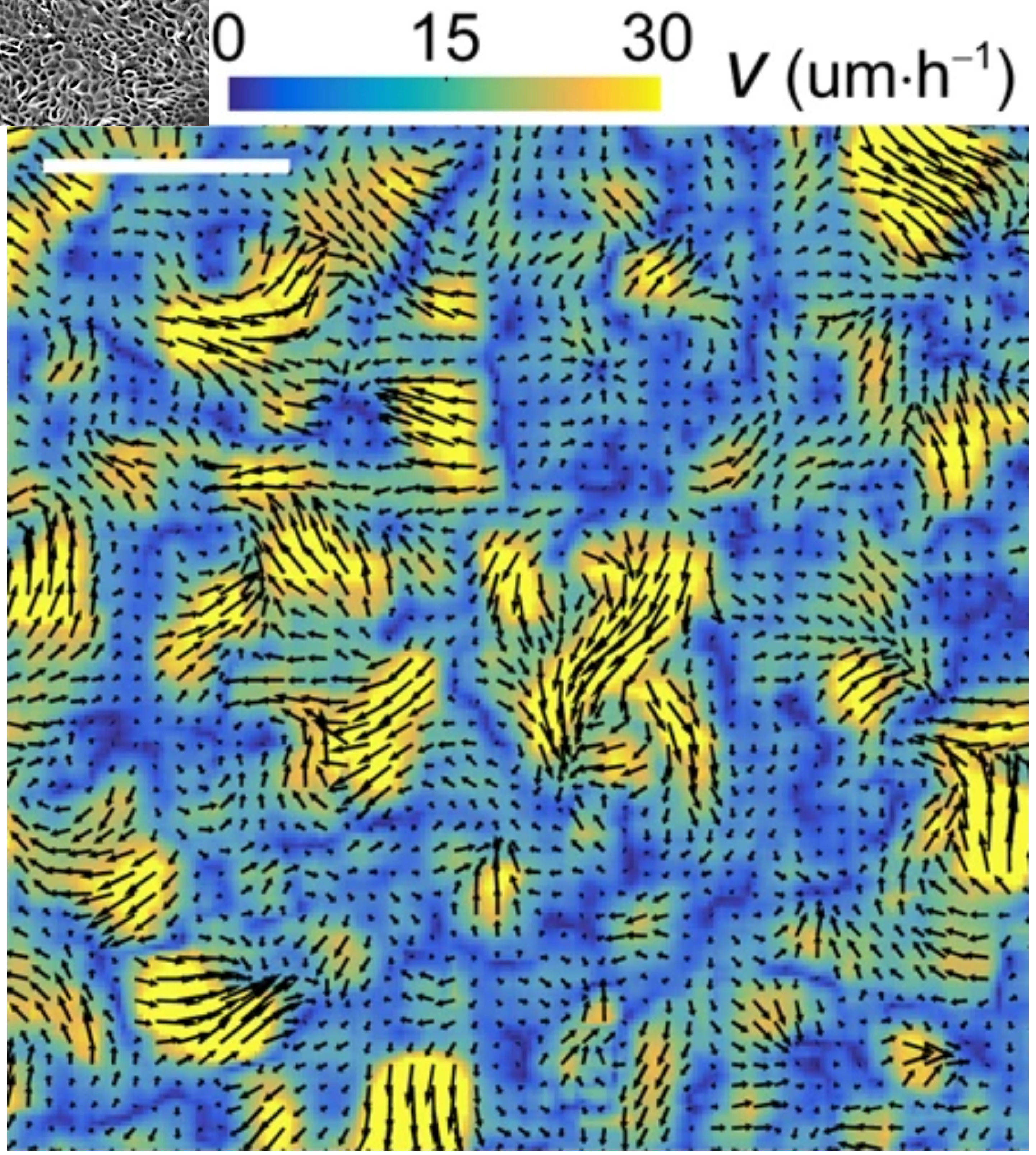

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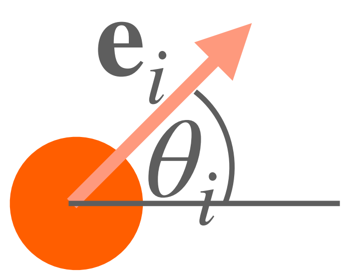

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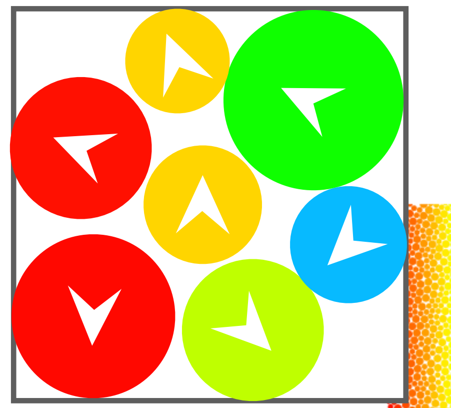

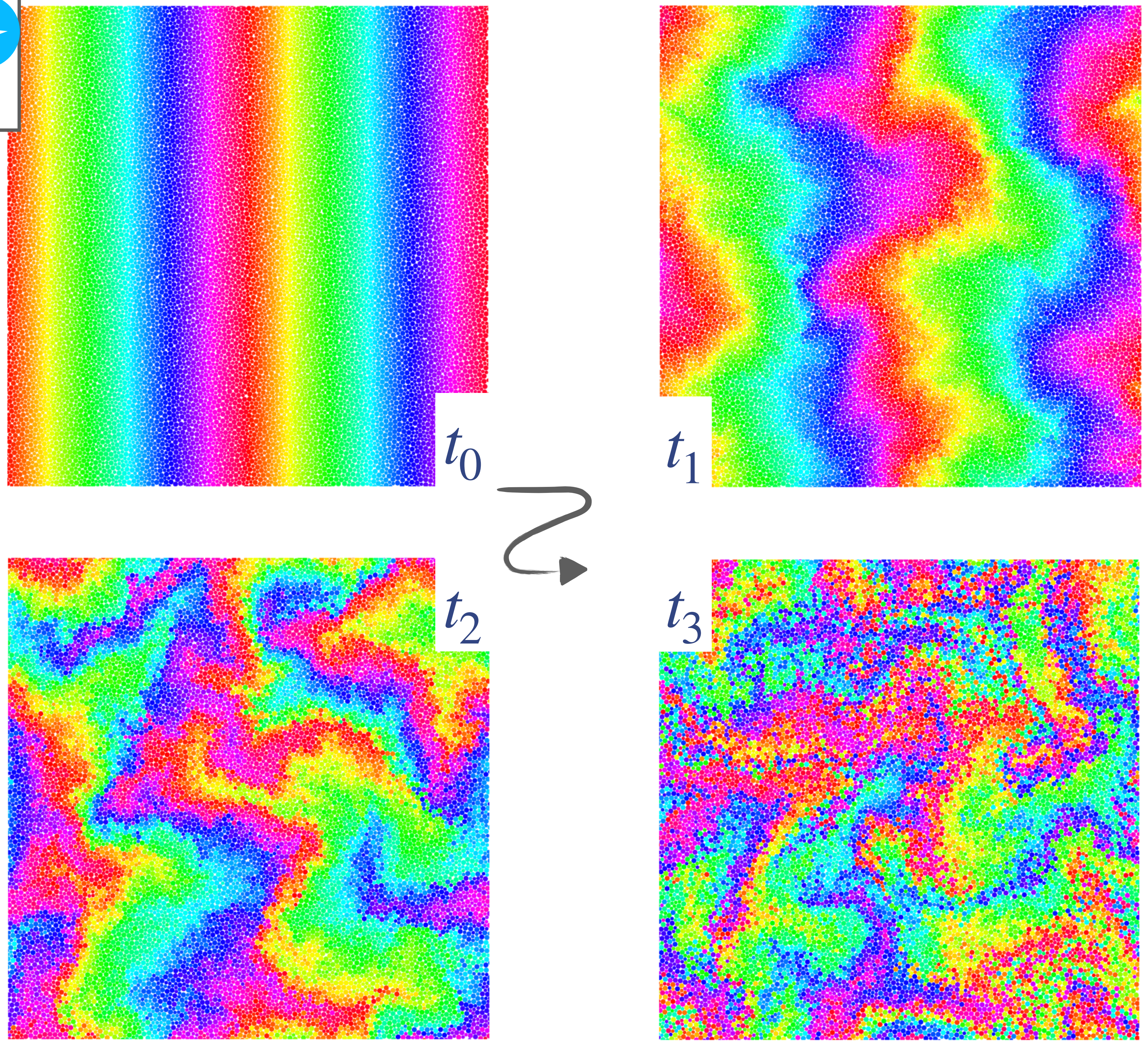

YE Keta, **J. Klamser**, RL Jack, L. Berthier, arXiv 2306.07172 (2023).

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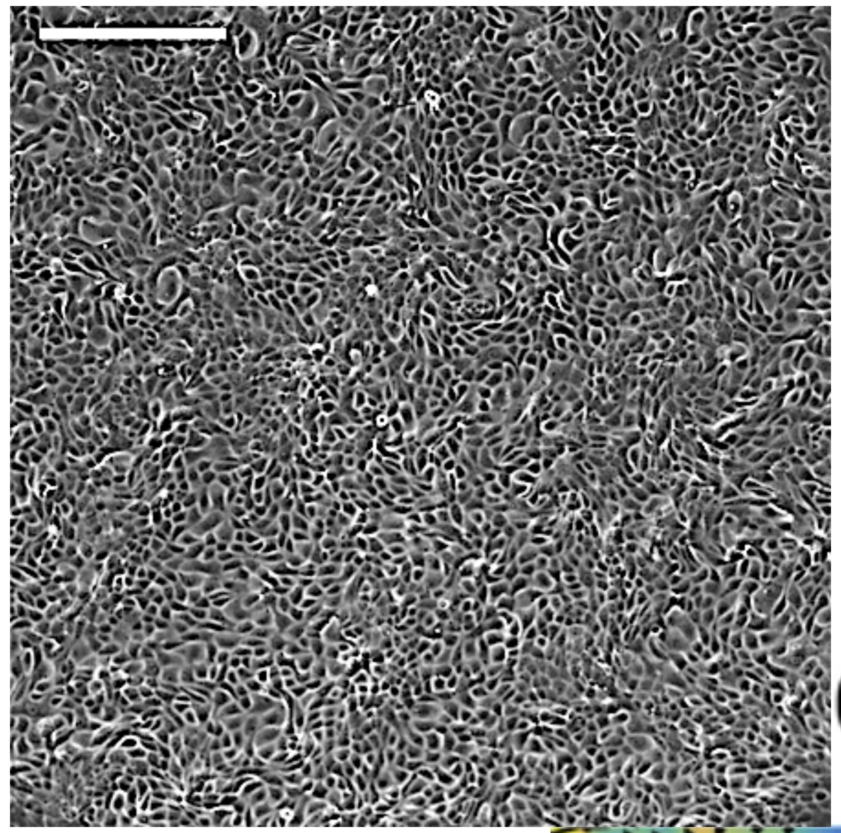

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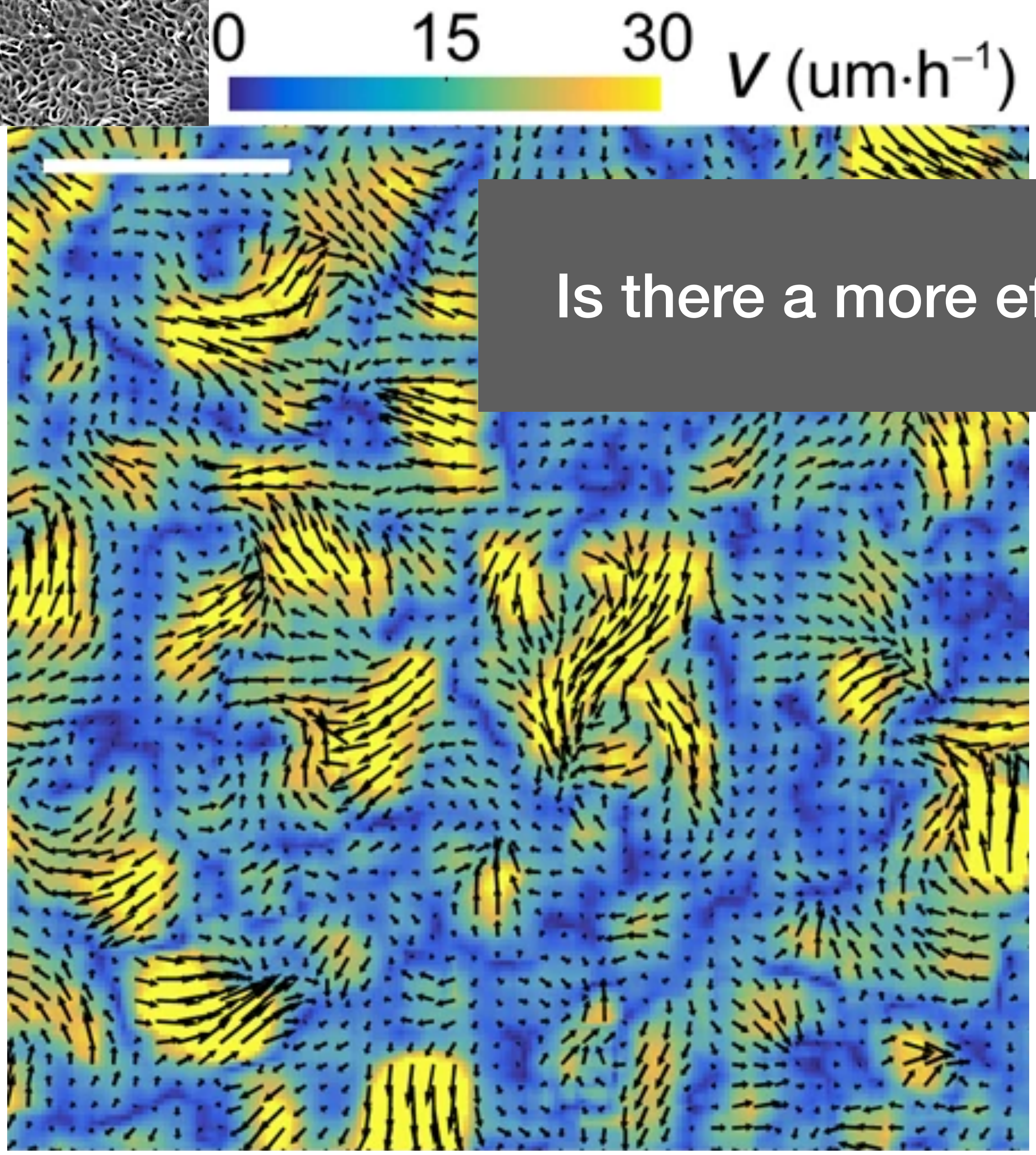

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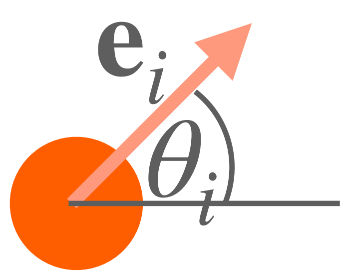

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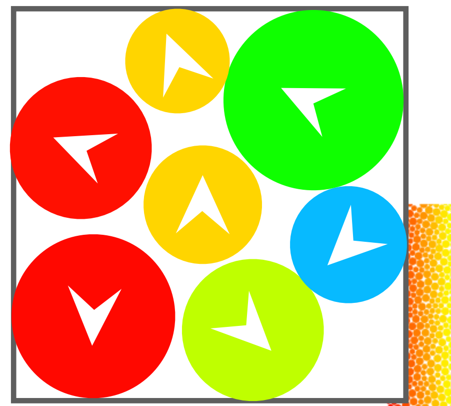

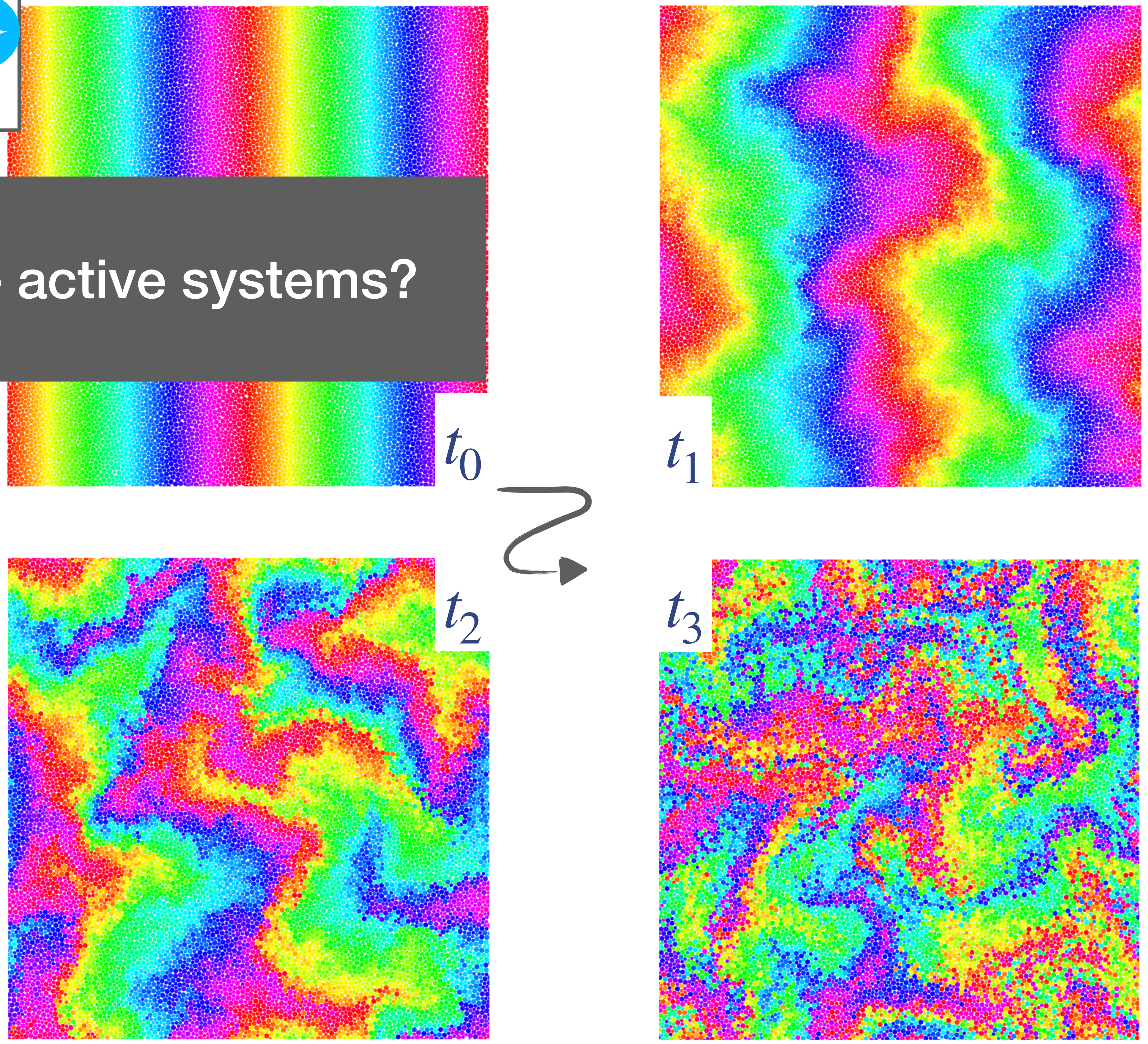

Is there a more efficient way to simulate active systems?

YE Keta, **J. Klamser**, RL Jack, L. Berthier, arXiv 2306.07172 (2023).

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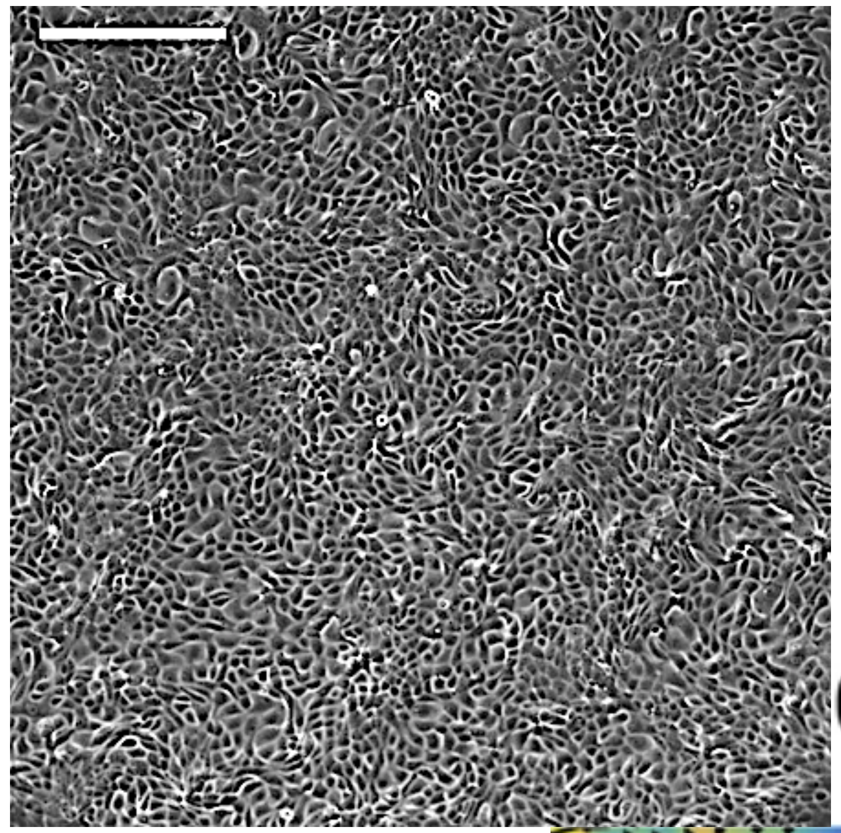

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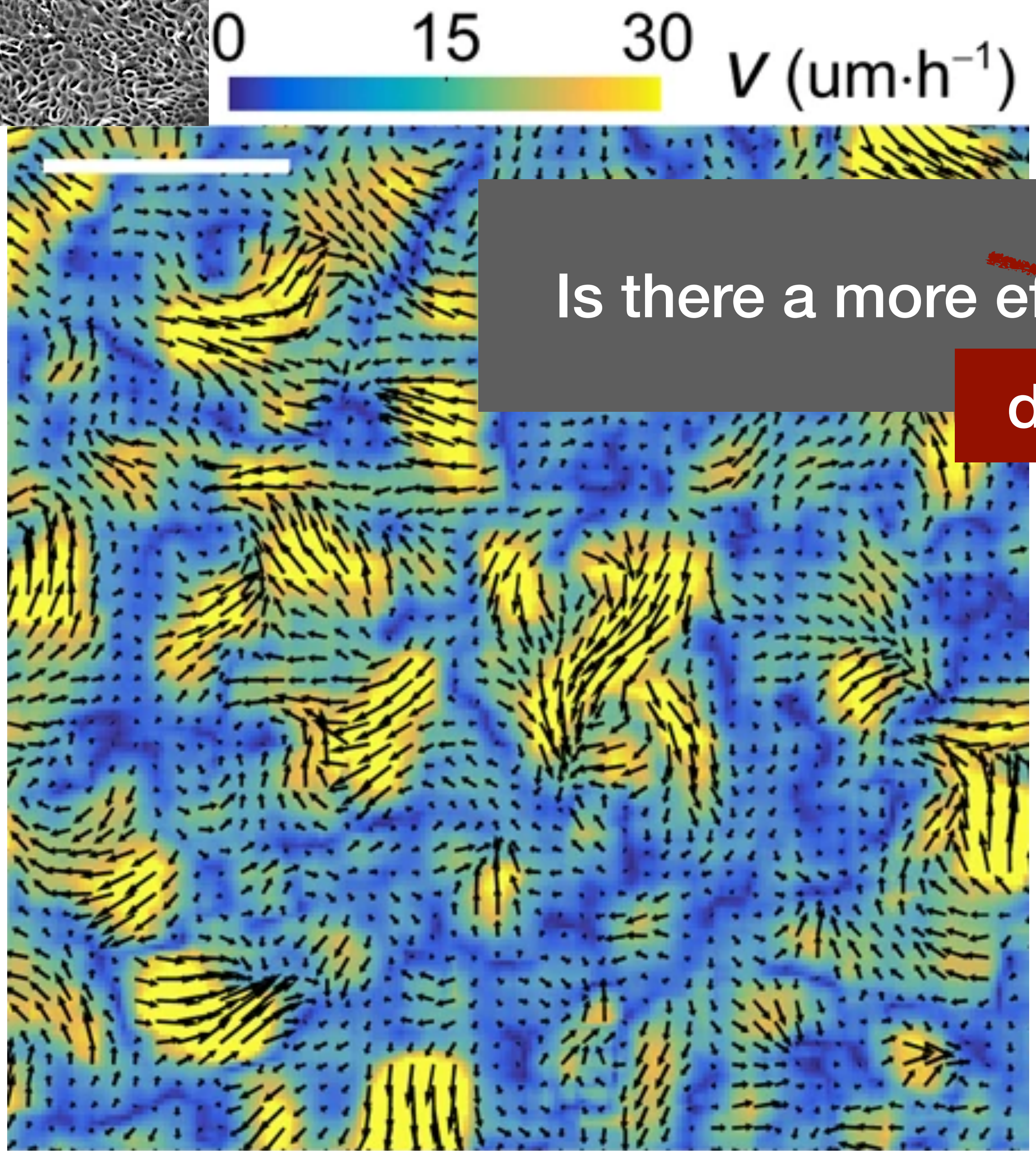

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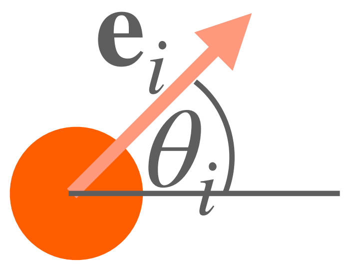

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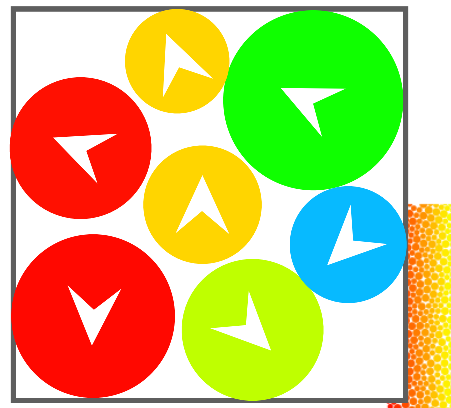

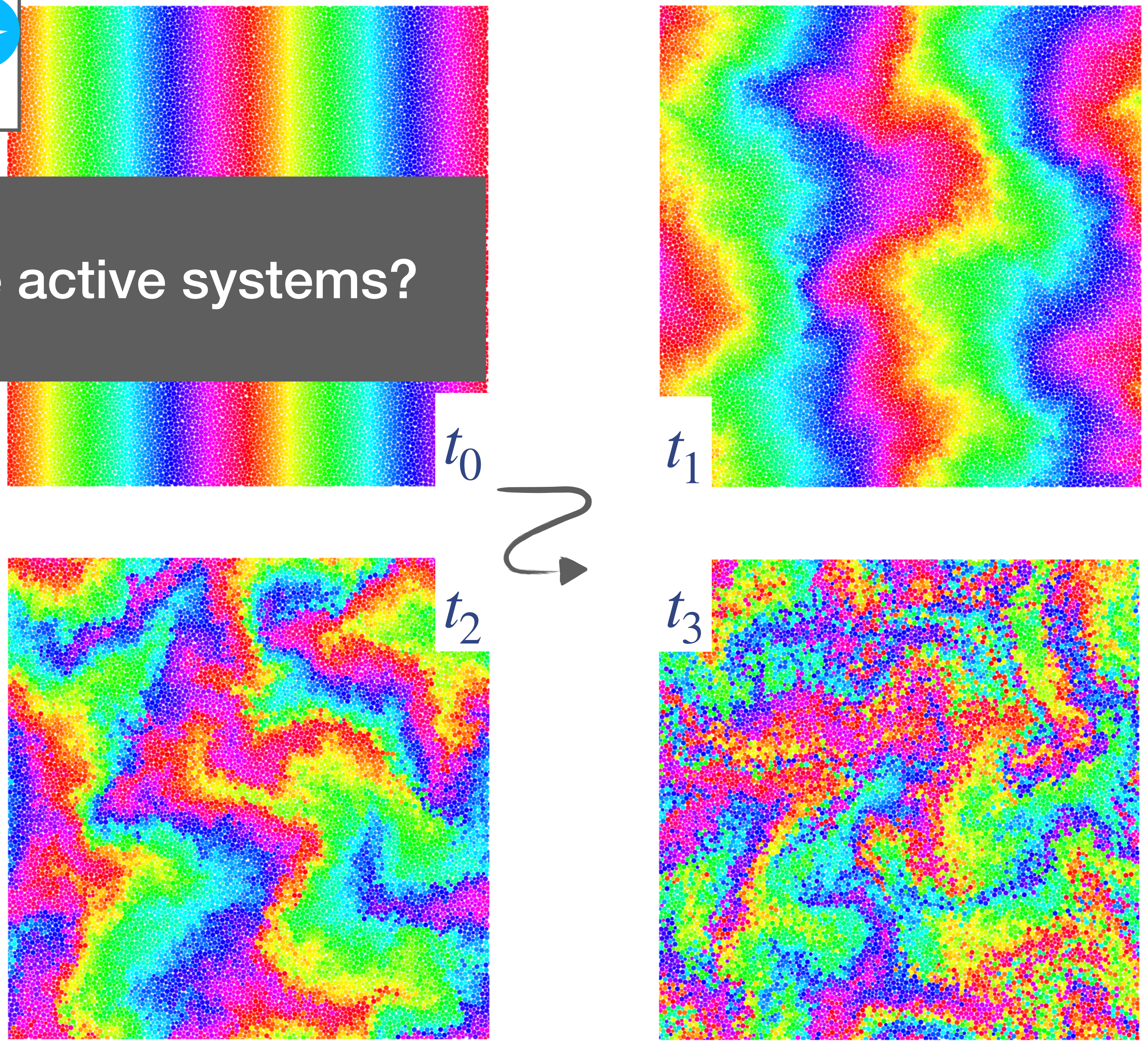

Is there a more ~~efficient~~ different way to simulate active systems?

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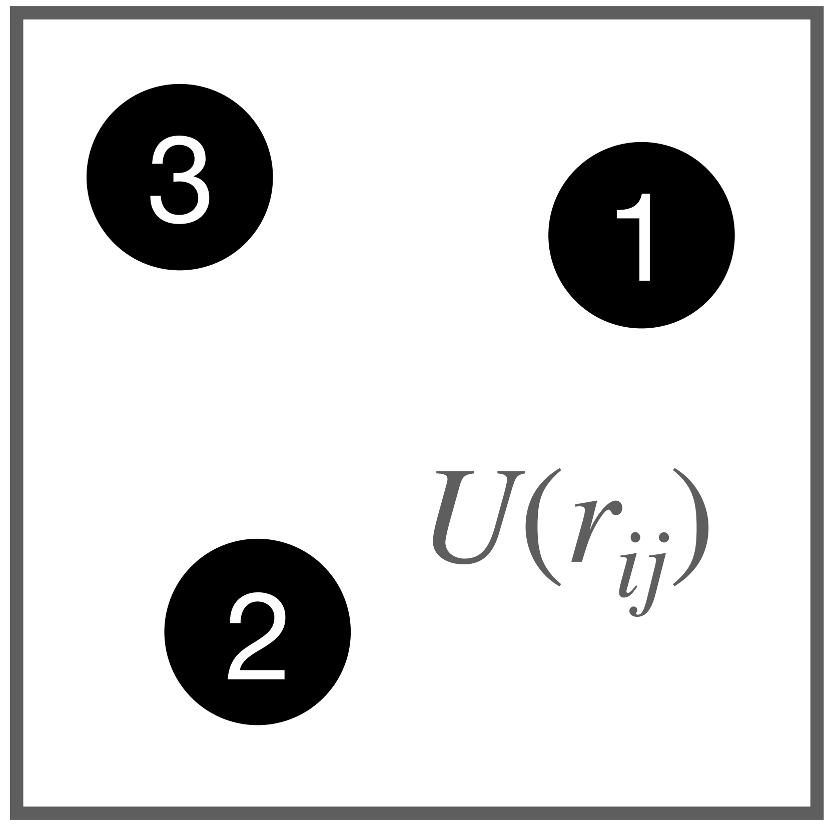
Monte Carlo for persistently moving particles - version 1.0

$C = \{\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\}$



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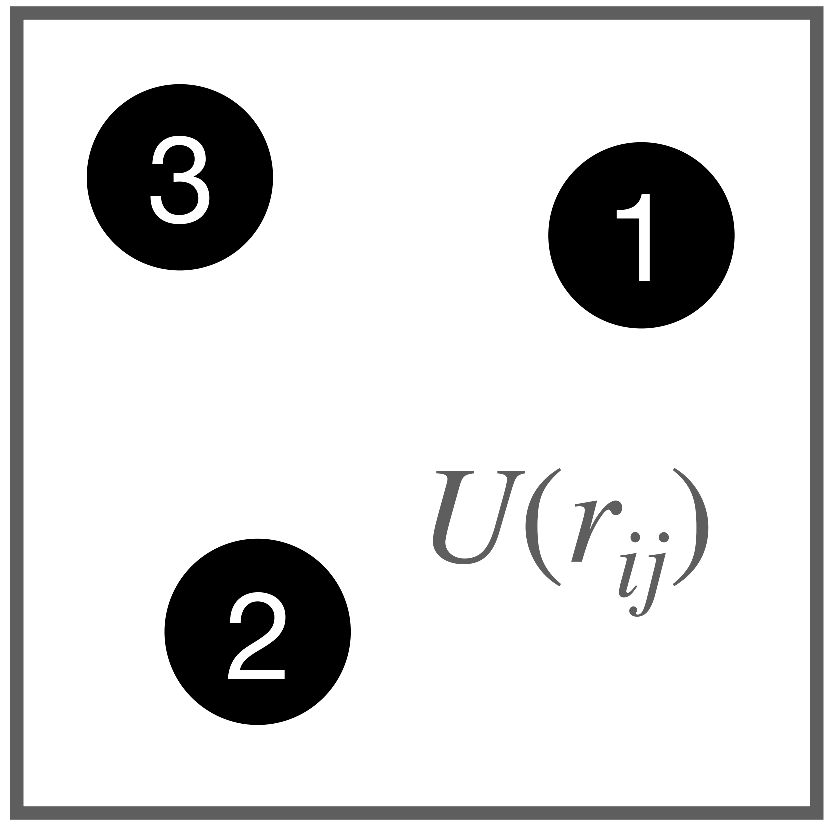

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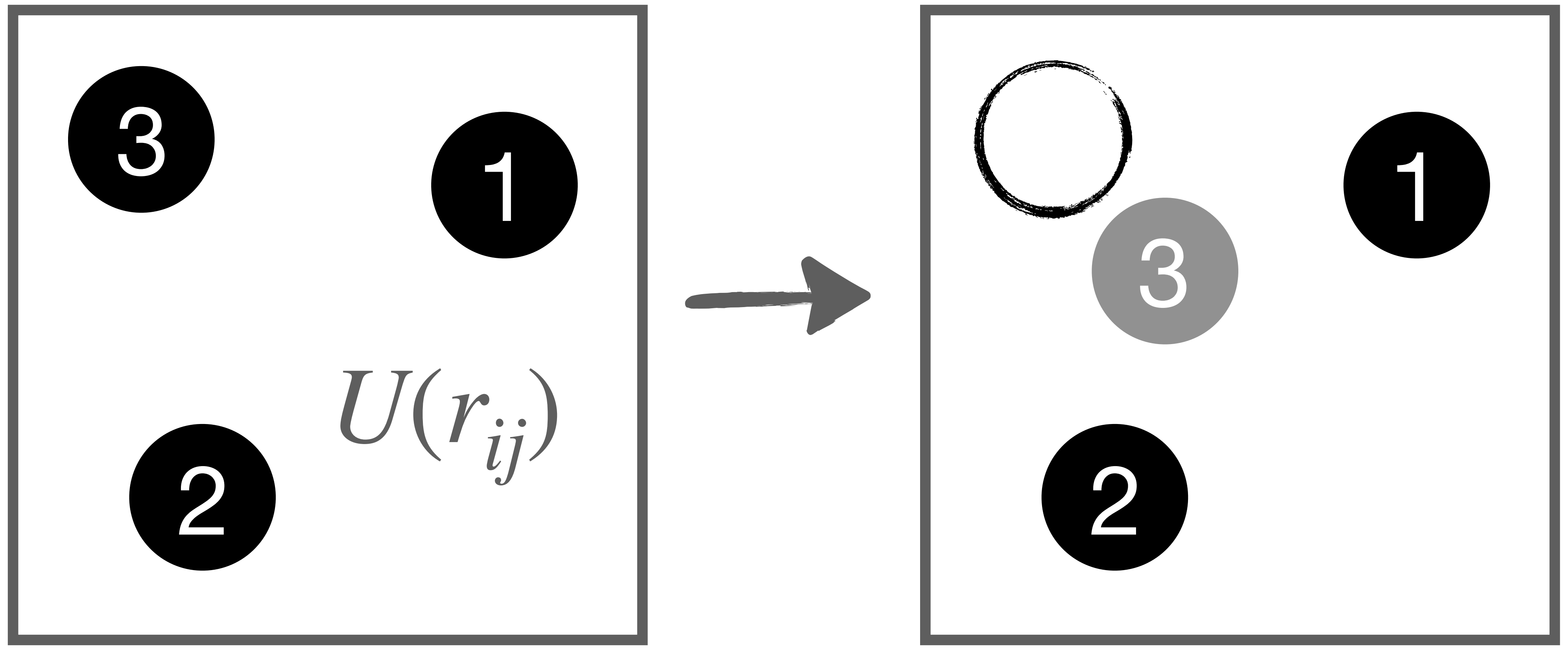

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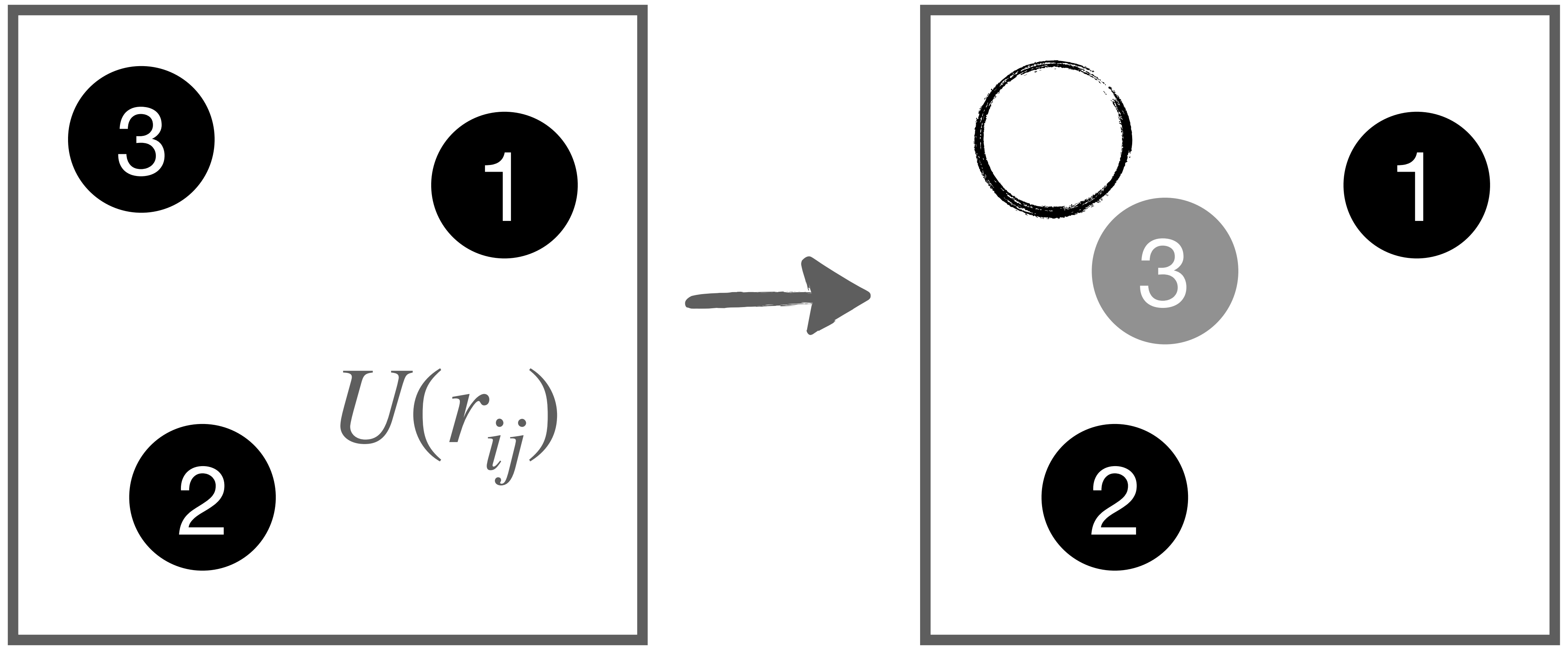

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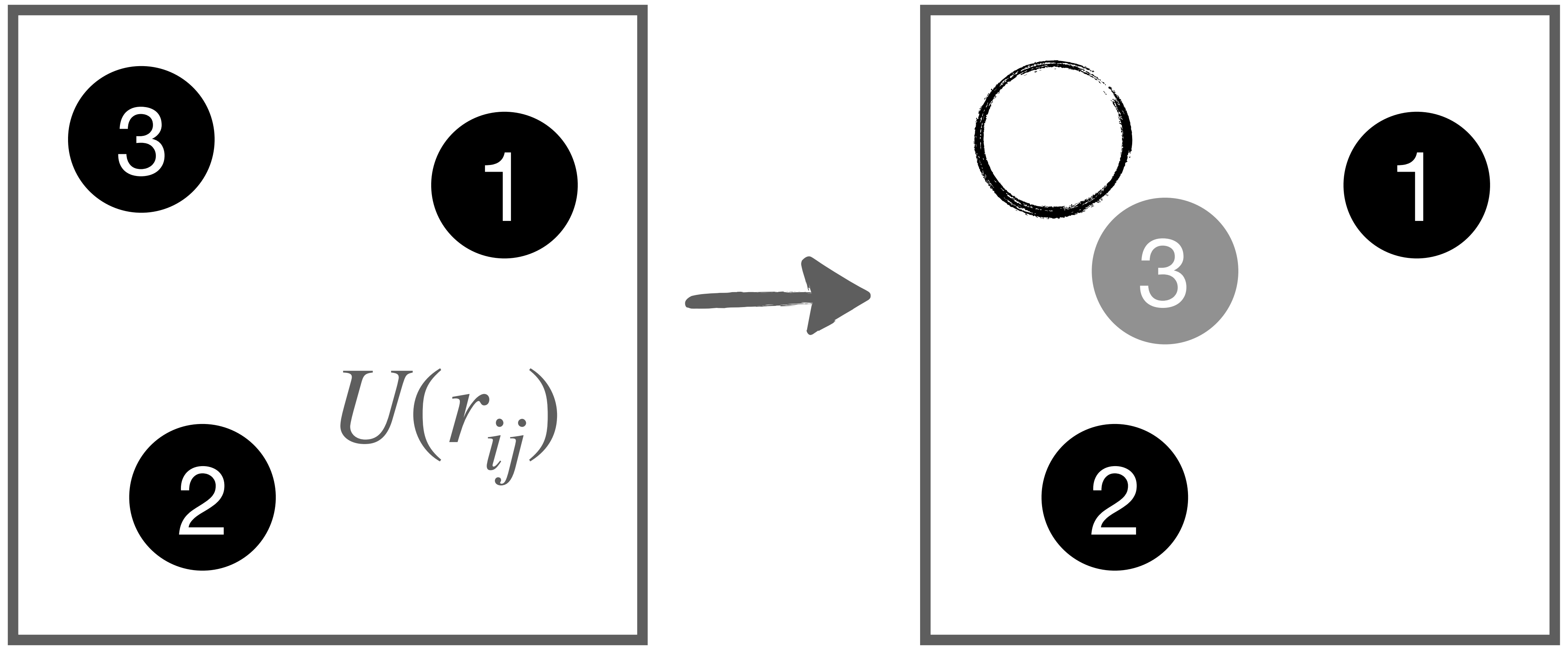

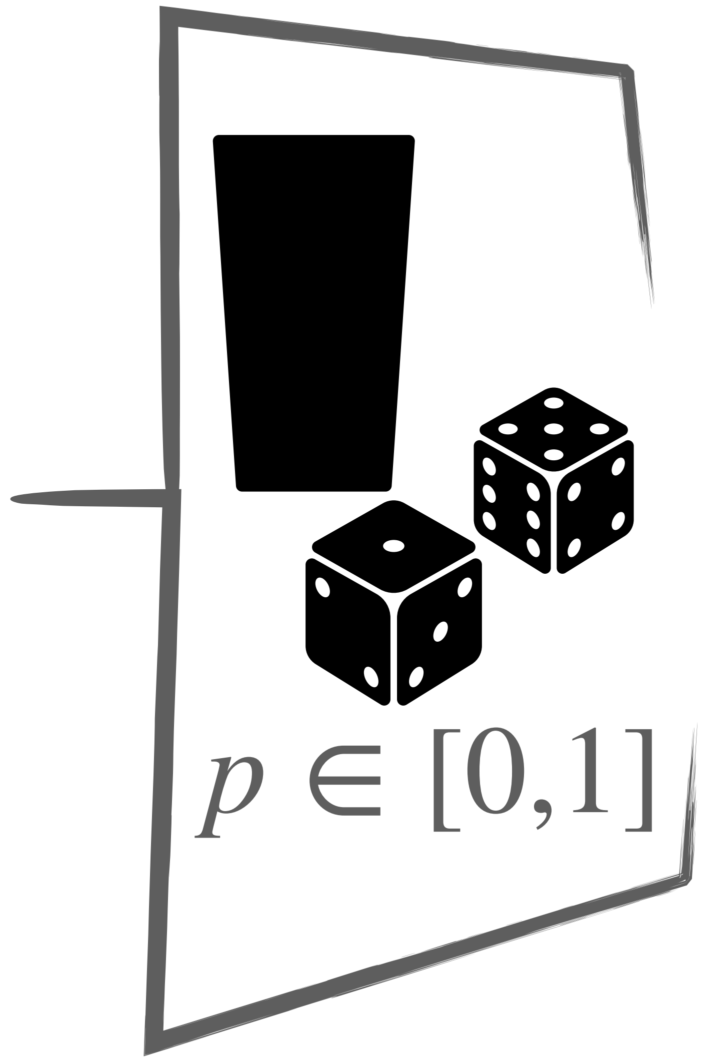

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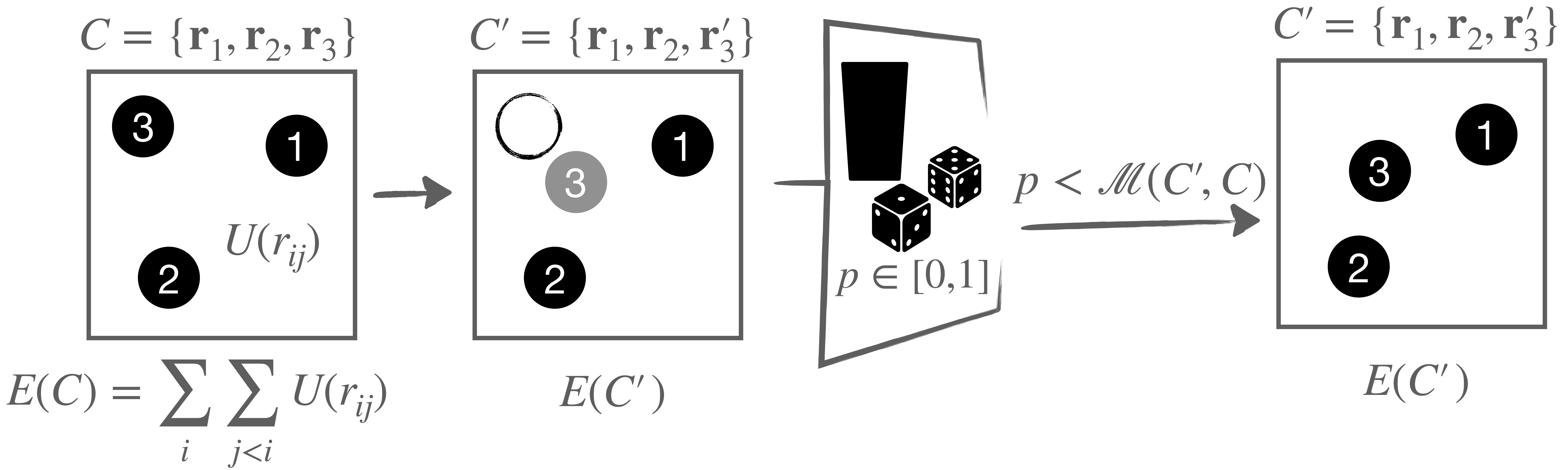

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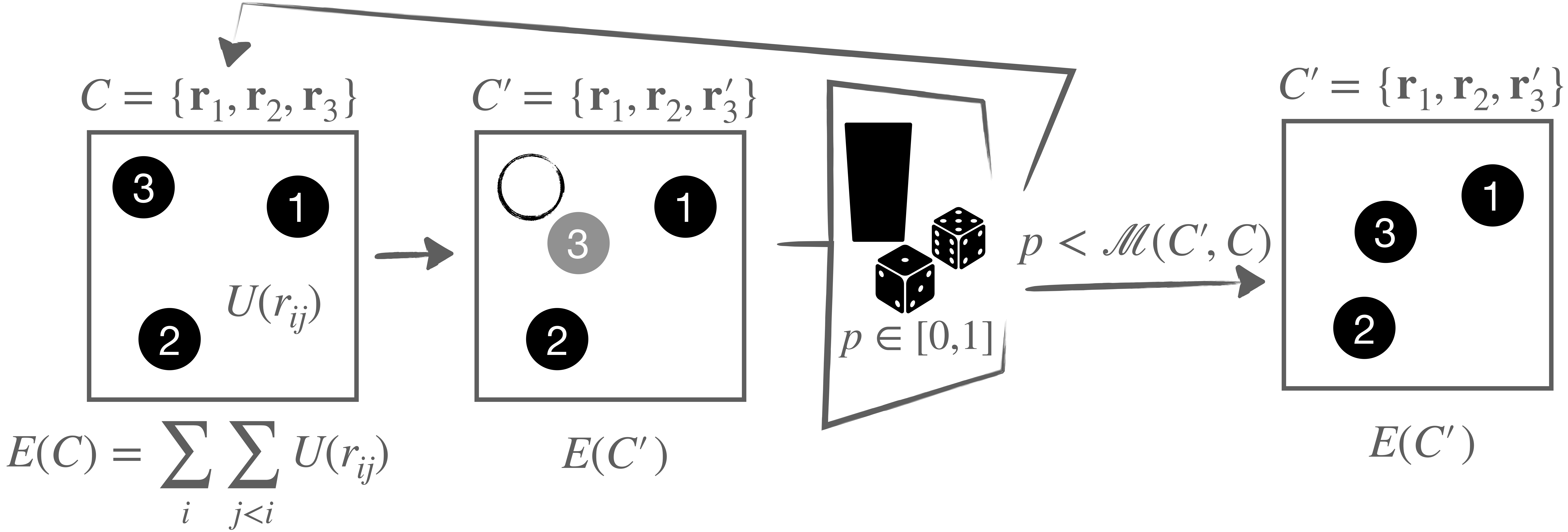

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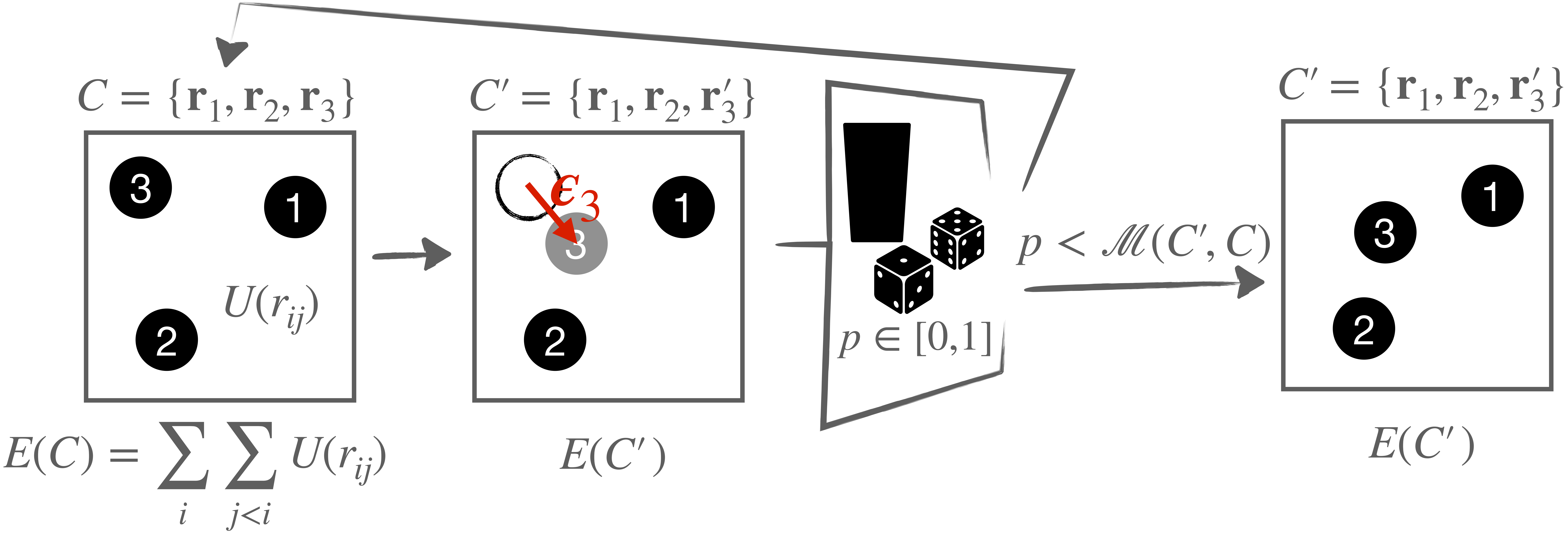

Equilibrium Monte Carlo: $G(\epsilon_i)$ = flat measure

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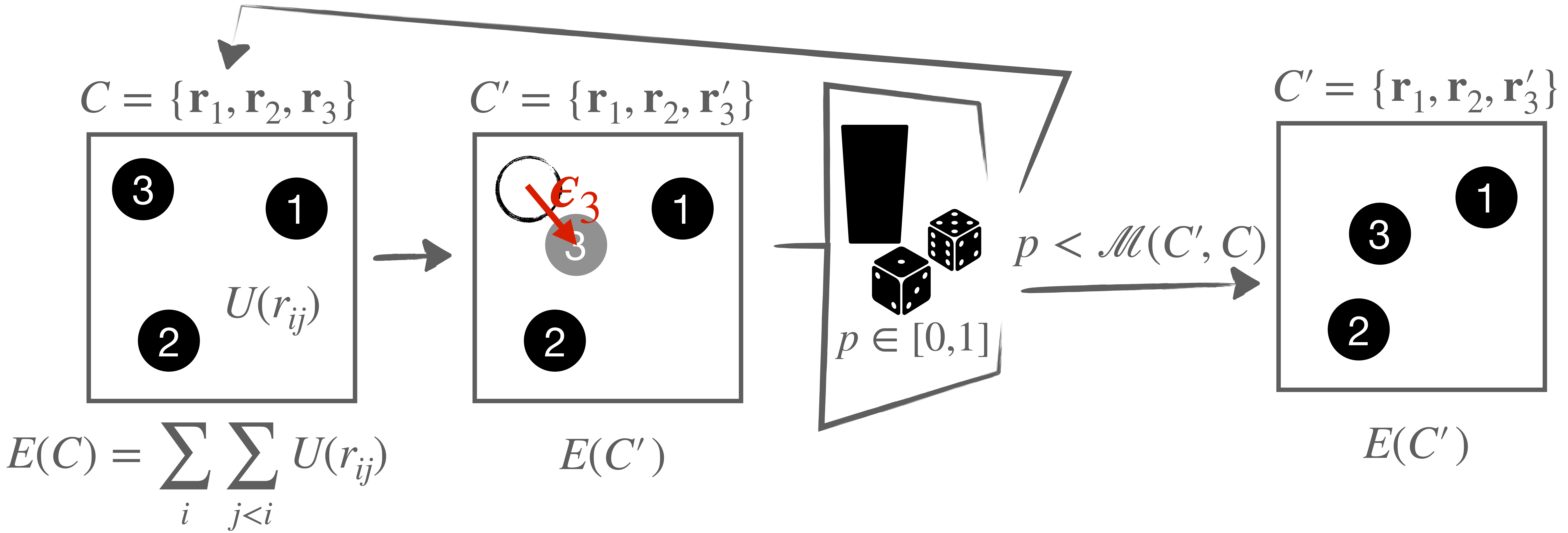

Equilibrium Monte Carlo: $G(\epsilon_i)$ = flat measure

Active kinetic MC: $g(\epsilon_i \to \epsilon'_i)$, time correlated such that $\epsilon'_i \simeq \epsilon_i$

λ - persistence length

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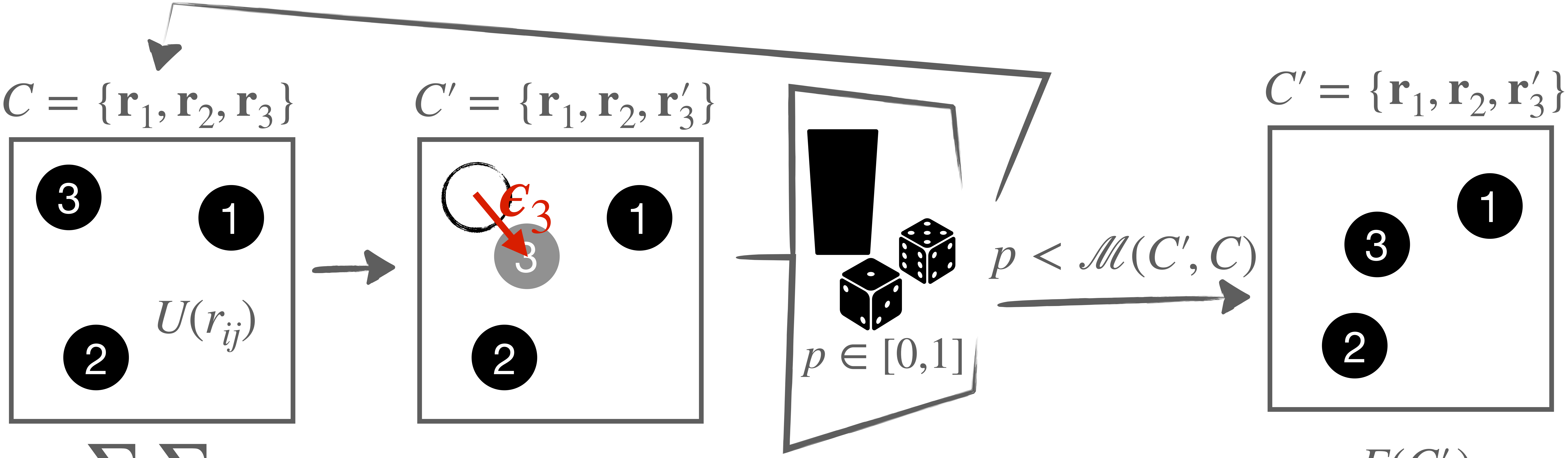

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Collective behaviour comparable with conventional active matter models ?

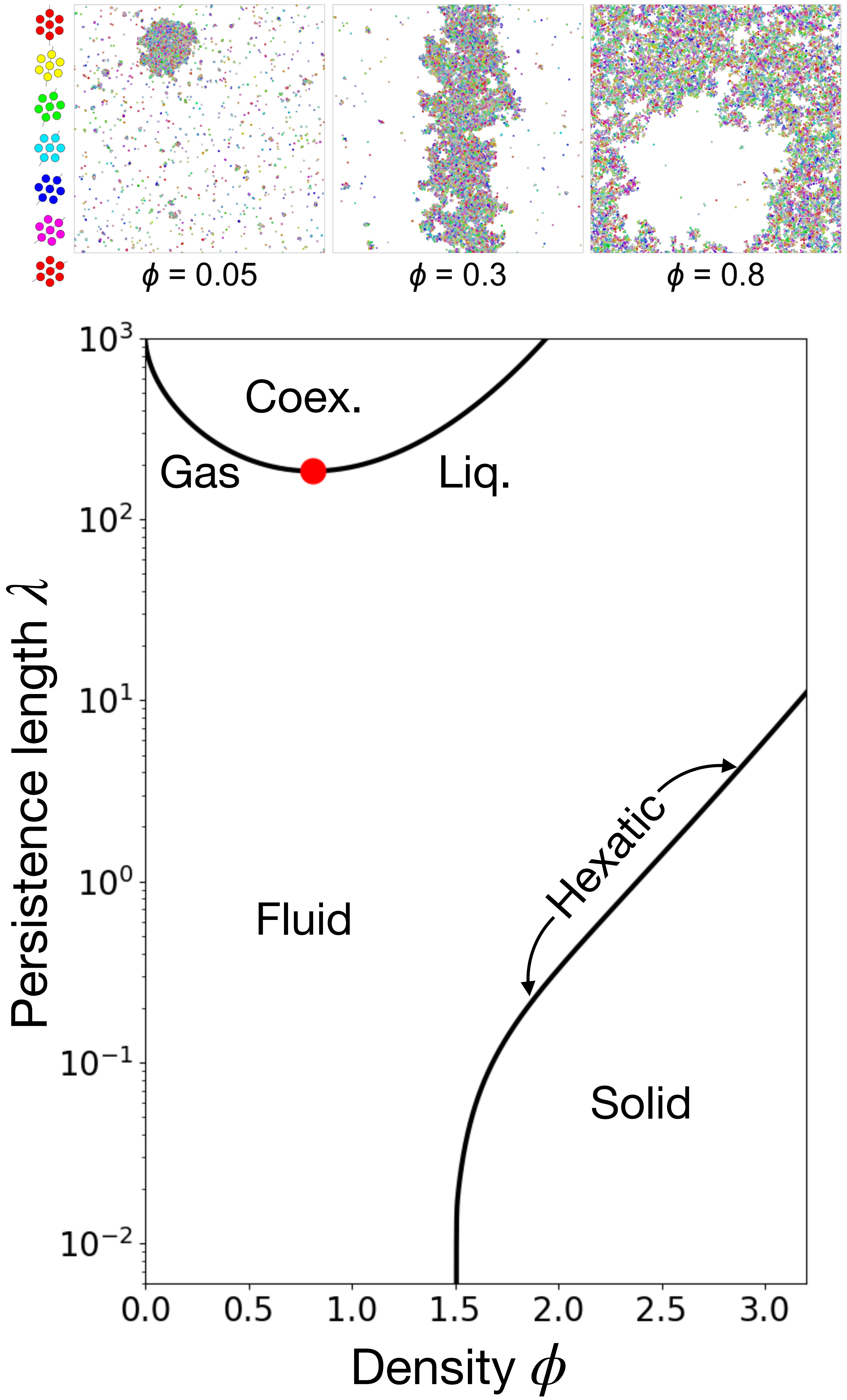
- D. Levis, L. Berthier, Phys. Rev. E (2014).
- L. Berthier, Phys Rev Lett (2014).
- **J. Klamser**, S. Kapfer, W. Krauth, Nat Commun (2018).
- **J. Klamser**, S. Kapfer, W. Krauth, J Chem Phys (2019).

Equilibrium Monte Carlo: $G(\epsilon_i)$ = flat measure

Active kinetic MC: $g(\epsilon_i \to \epsilon'_i)$, time correlated such that $\epsilon'_i \simeq \epsilon_i$

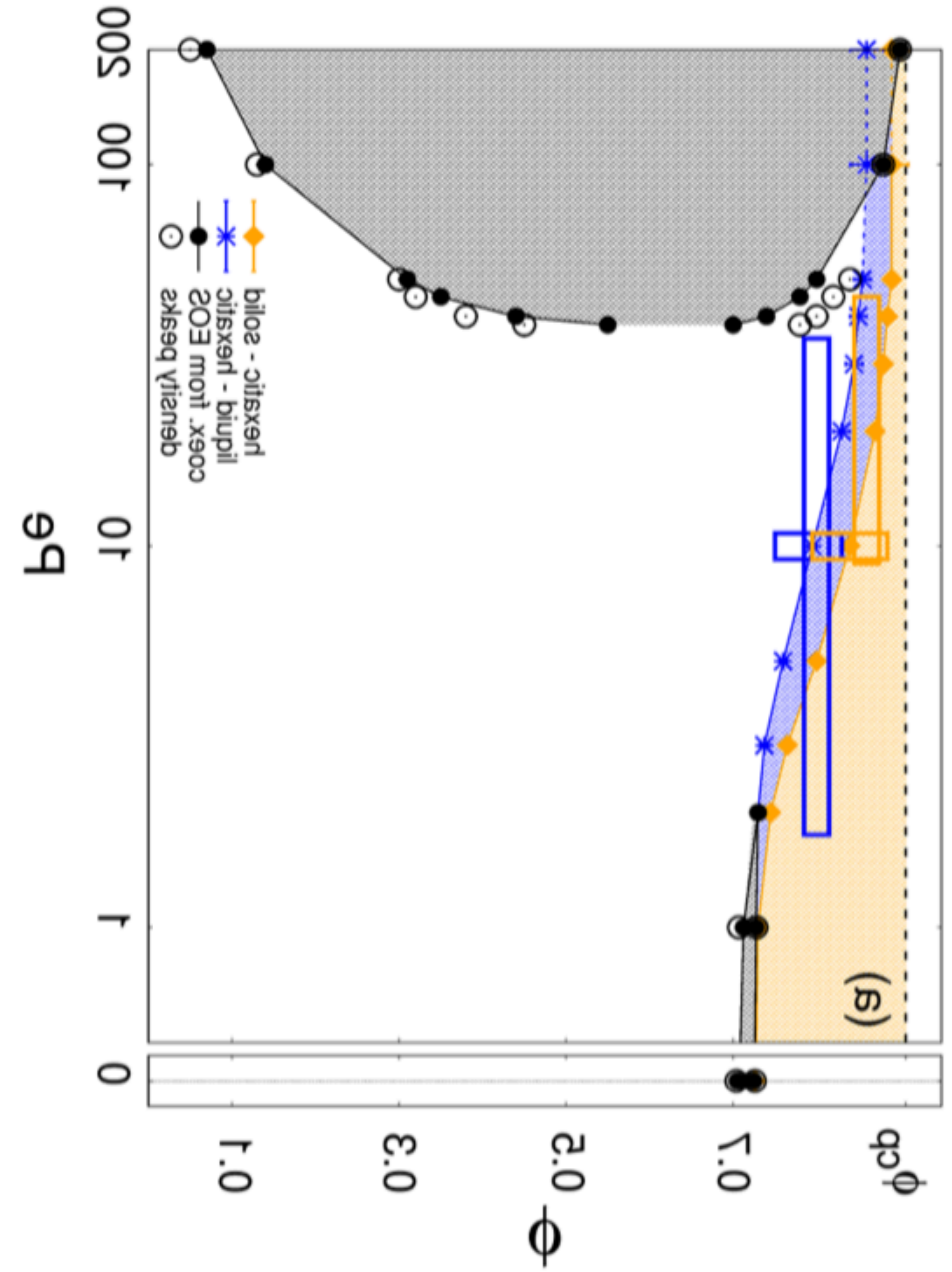
λ - persistence length

Active Kinetic Monte Carlo

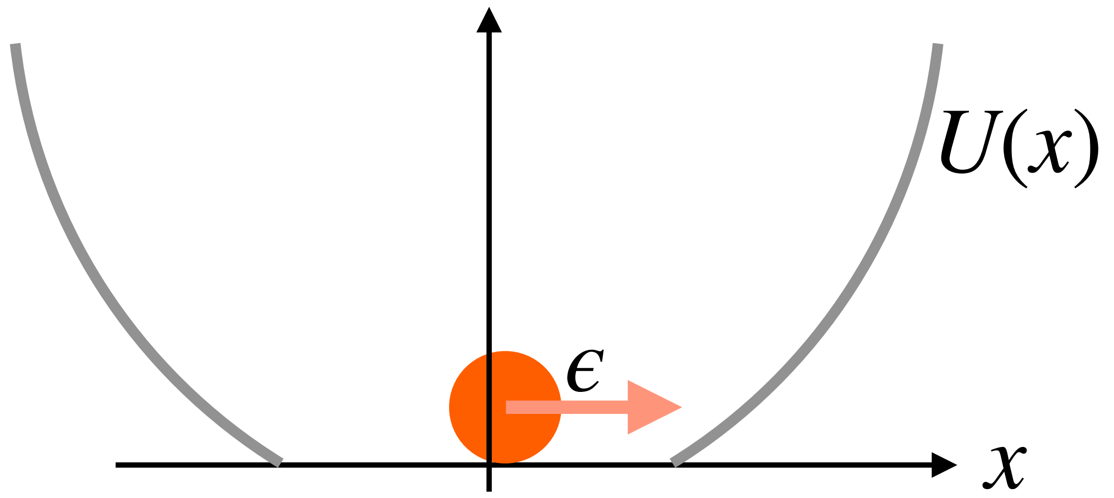


J. Klamser, S. Kapfer, W. Krauth, Nat Commun (2018).

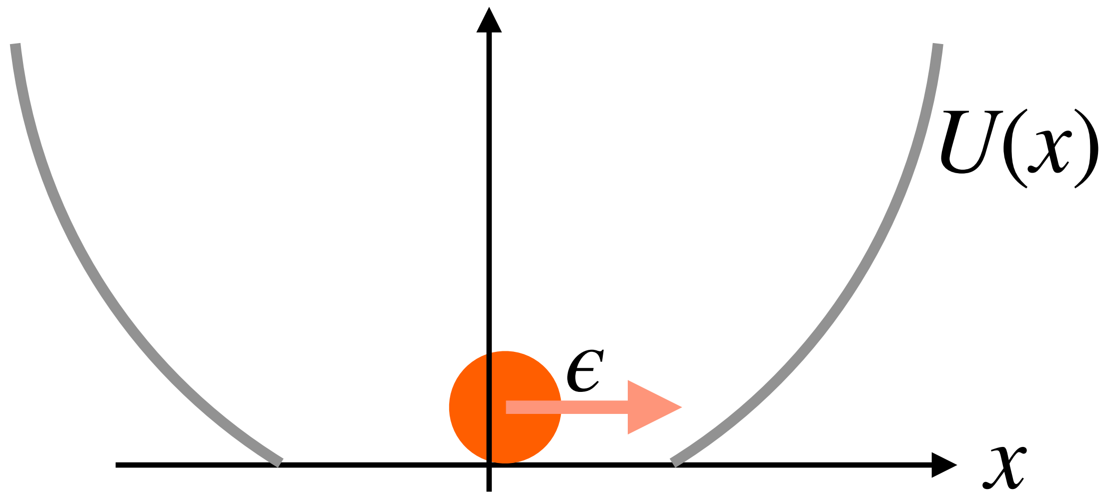
Active Brownian Particles



P. Digregorio, D. Levis, A. Suma, L. F. Cugliandolo, G. Gonnella, I. Pagonabarraga, Phys Rev Lett (2018).

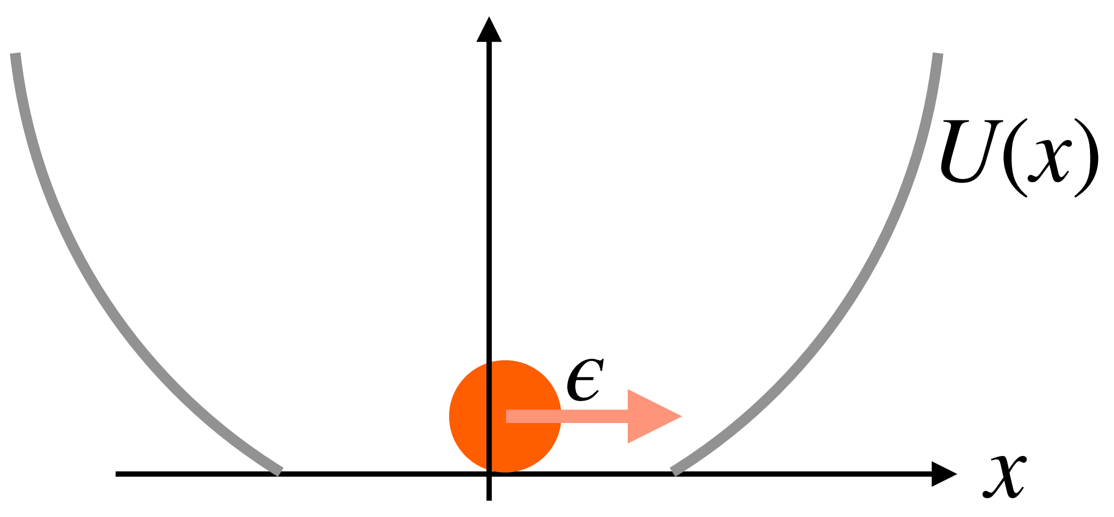


Continuous-time limit



Continuous-time limit

$$v = \frac{\epsilon}{dt} \quad t = n dt$$



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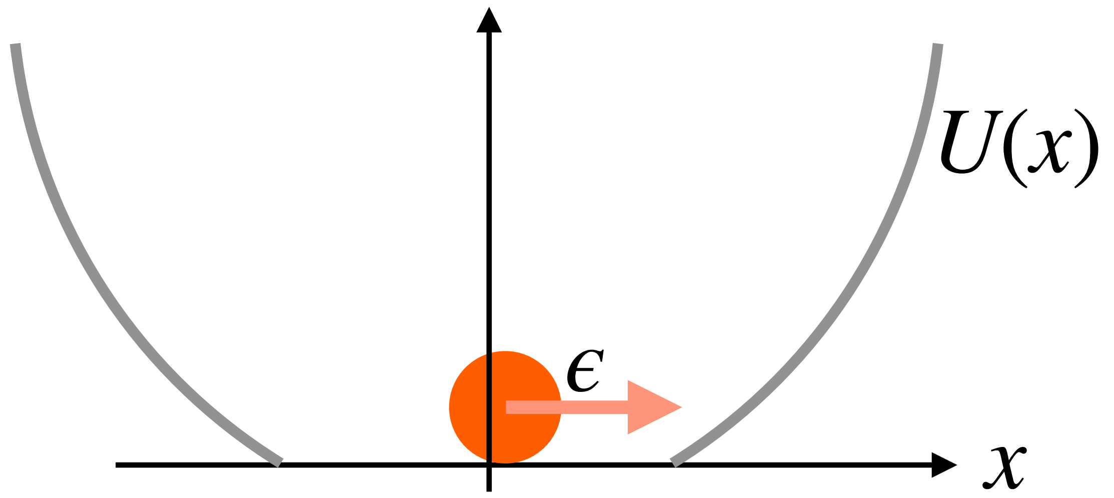
$dt \to 0$ with $v_0 = \text{const}$



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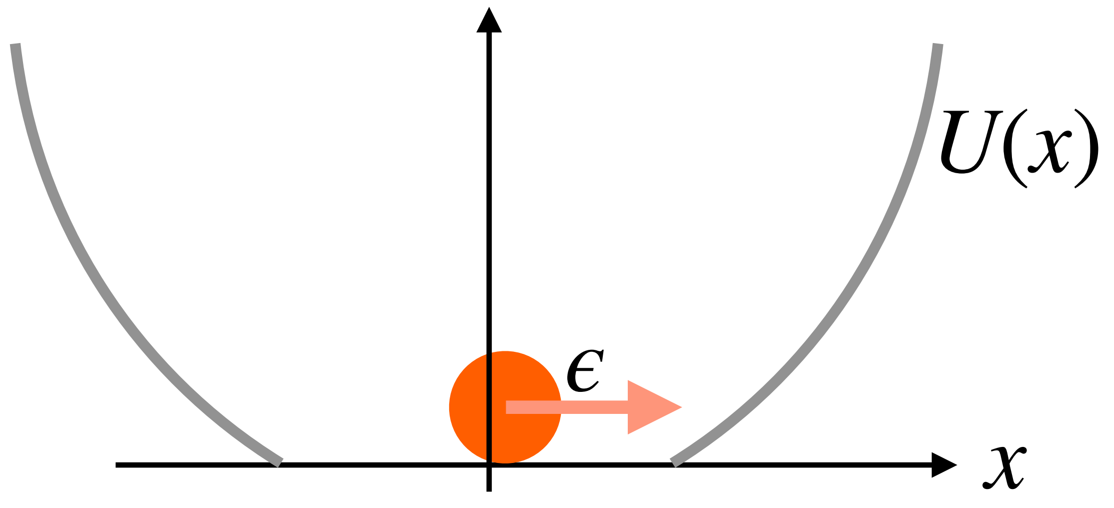

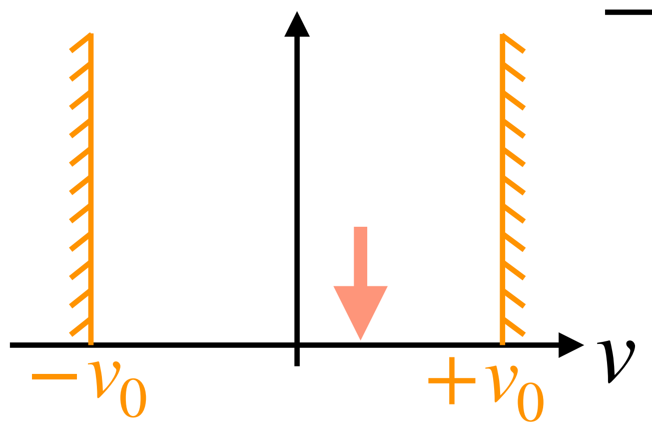

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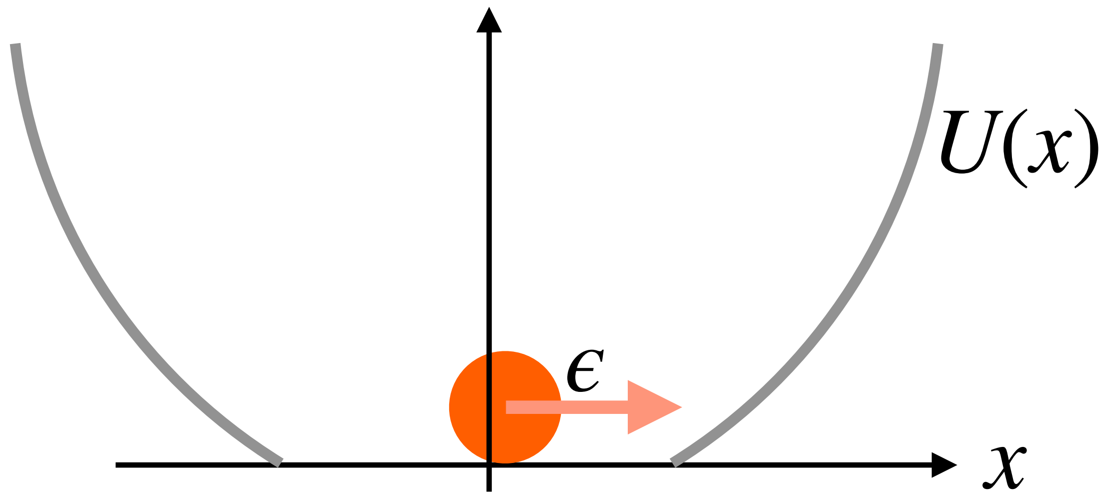

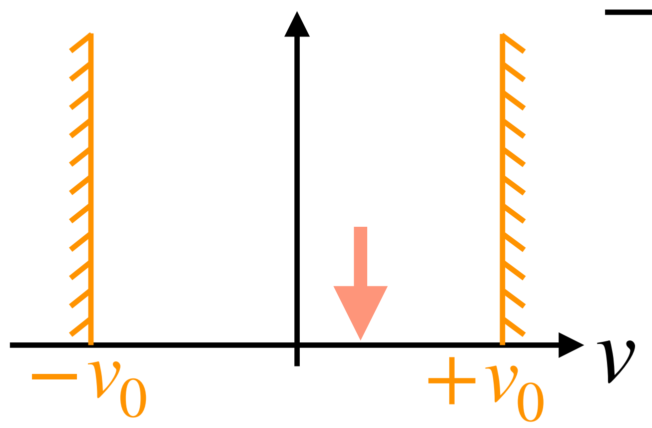

Continuous-time limit

$$v = \frac{\epsilon}{dt} \quad t = ndt \quad \langle \Delta v^2(t) \rangle = \sqrt{2D_v t}$$

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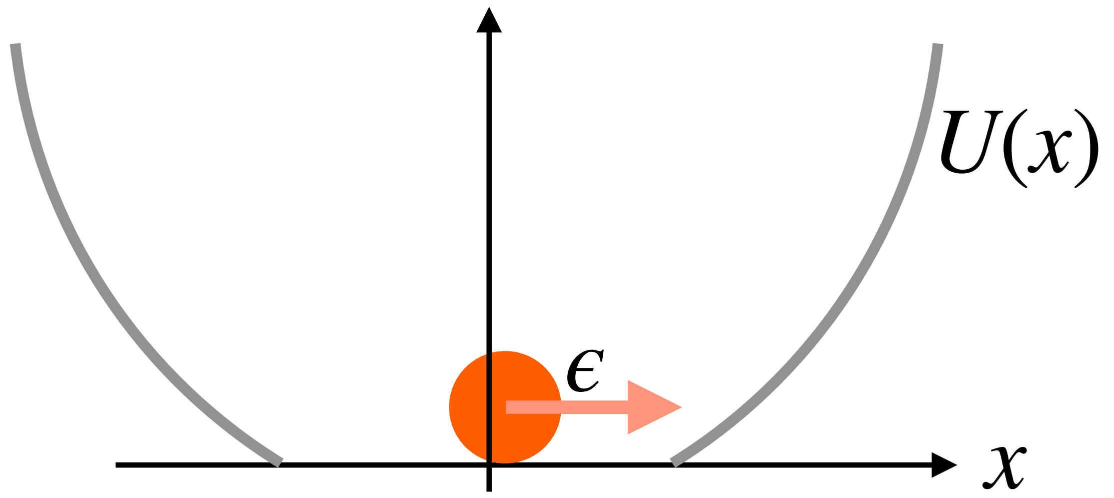

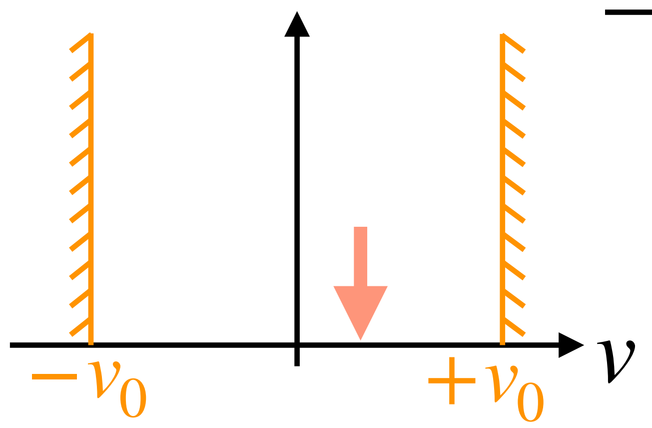

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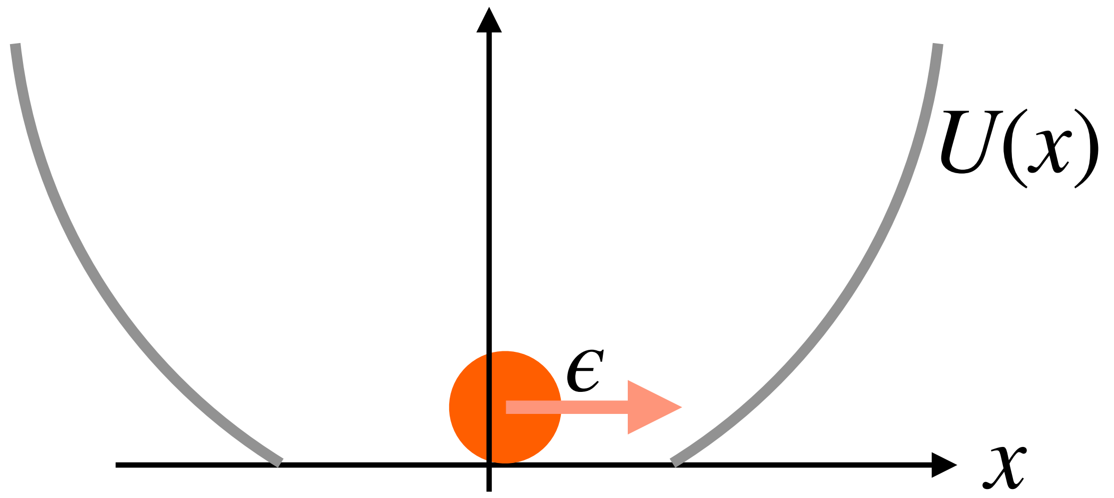

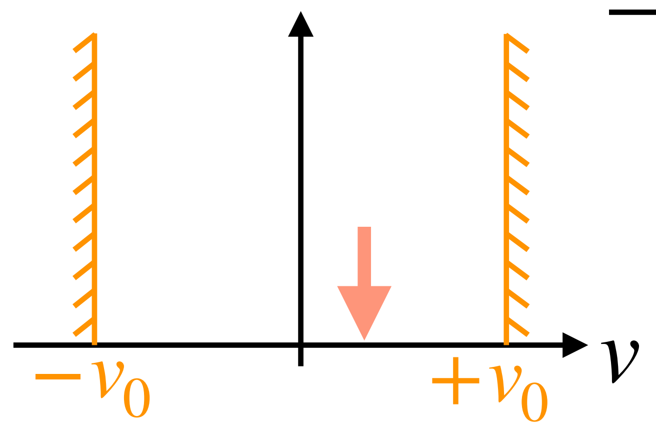

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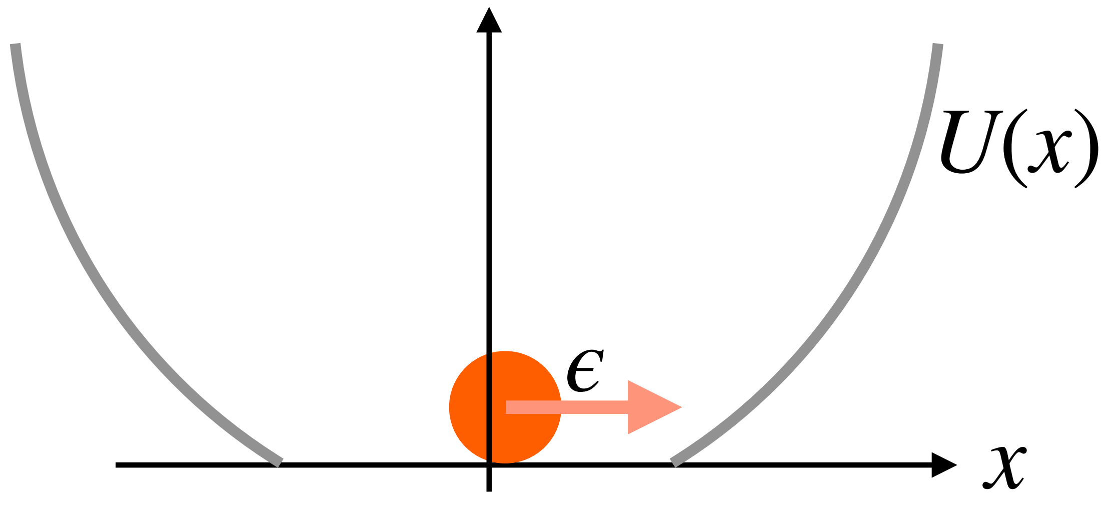

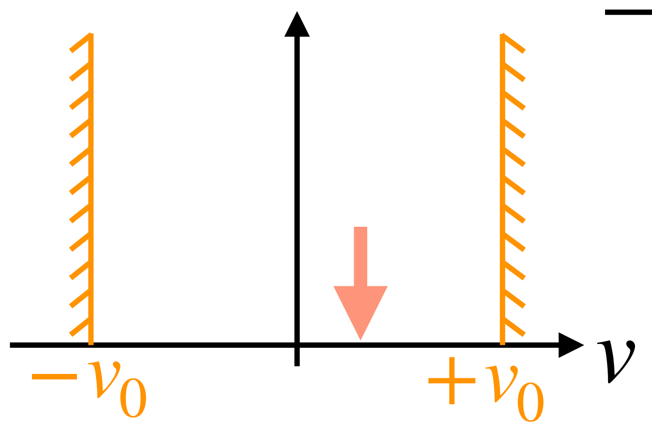

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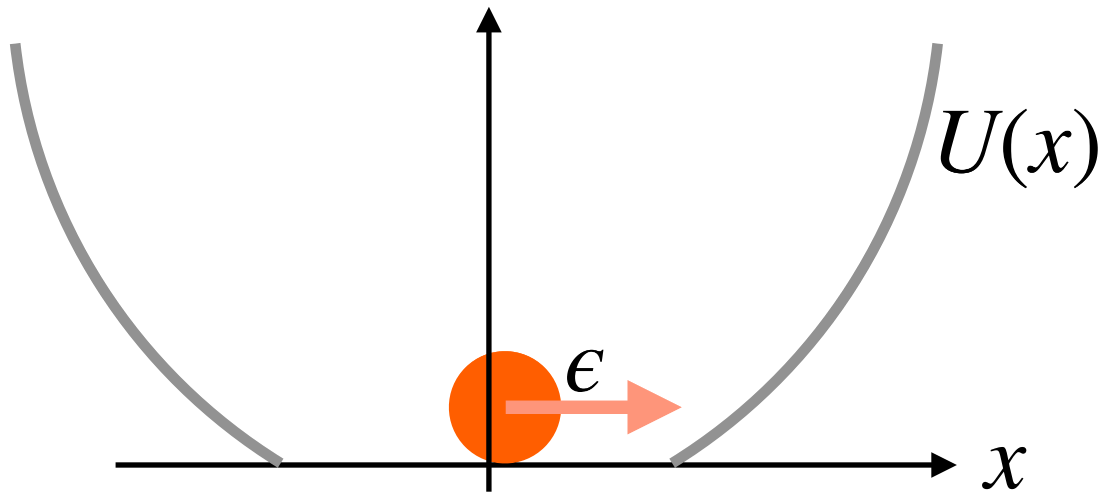

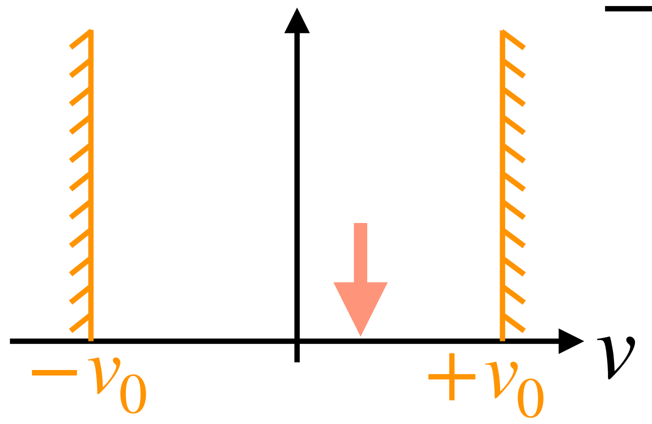

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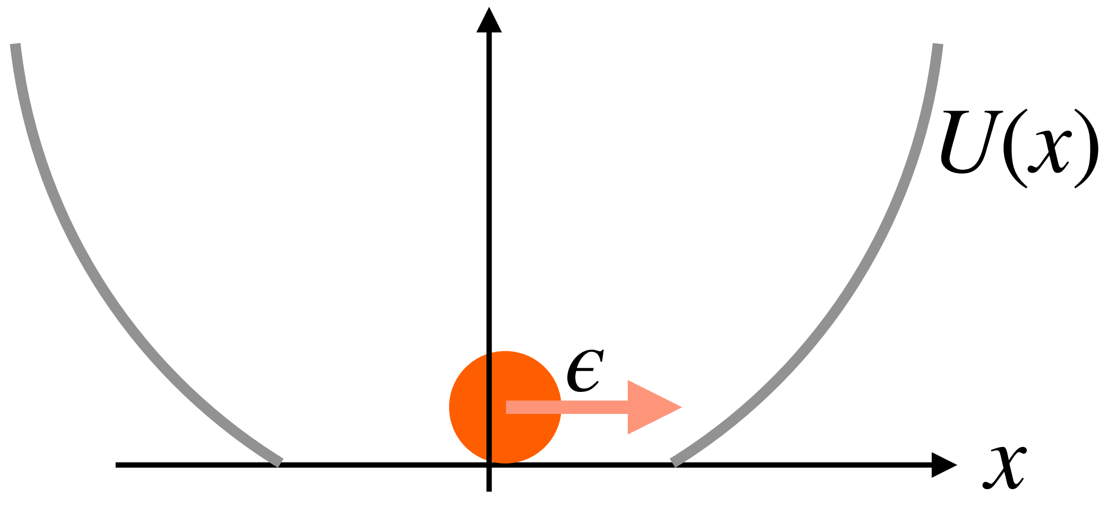
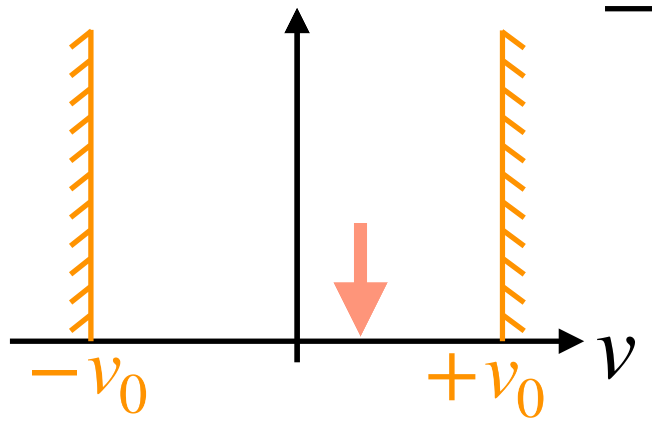
$$\frac{dx}{dt} = v \quad ; \quad \frac{dv}{dt} = \sqrt{2 D_v}\, \xi(t)$$





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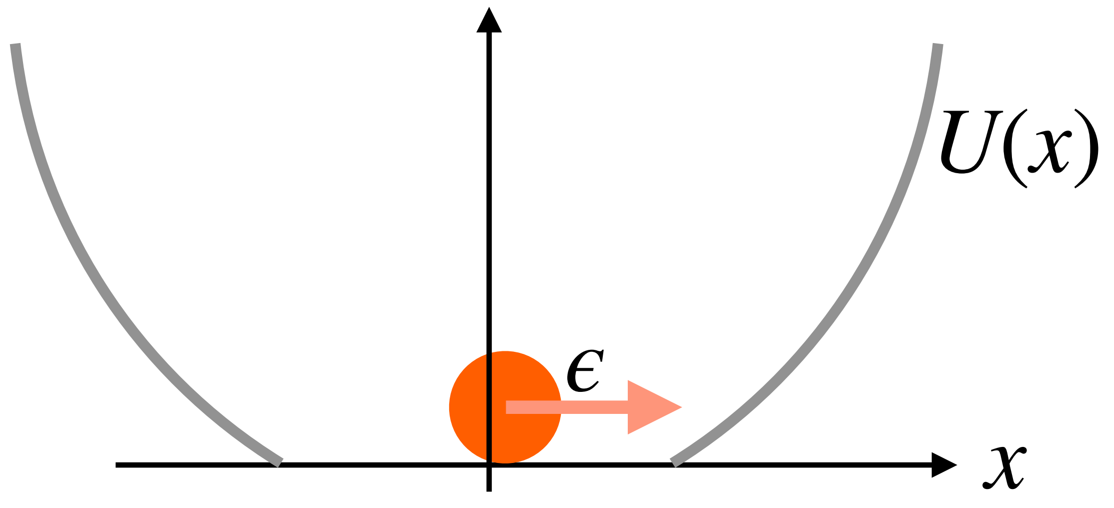

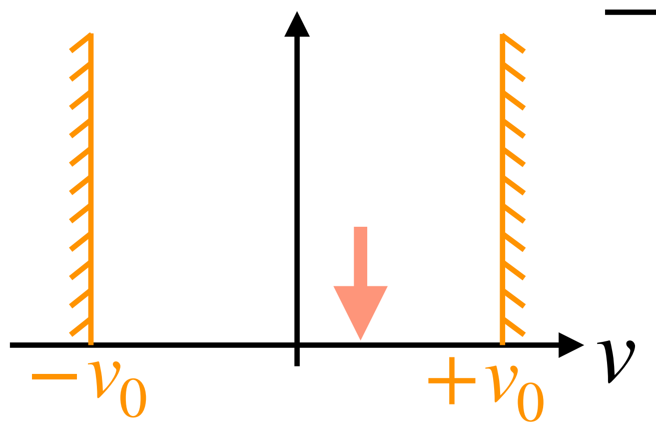

Continuous-time limit

$$v = \frac{\epsilon}{dt} \qquad t = n\,dt \qquad \langle \Delta v^2(t) \rangle = \sqrt{2D_v t}$$

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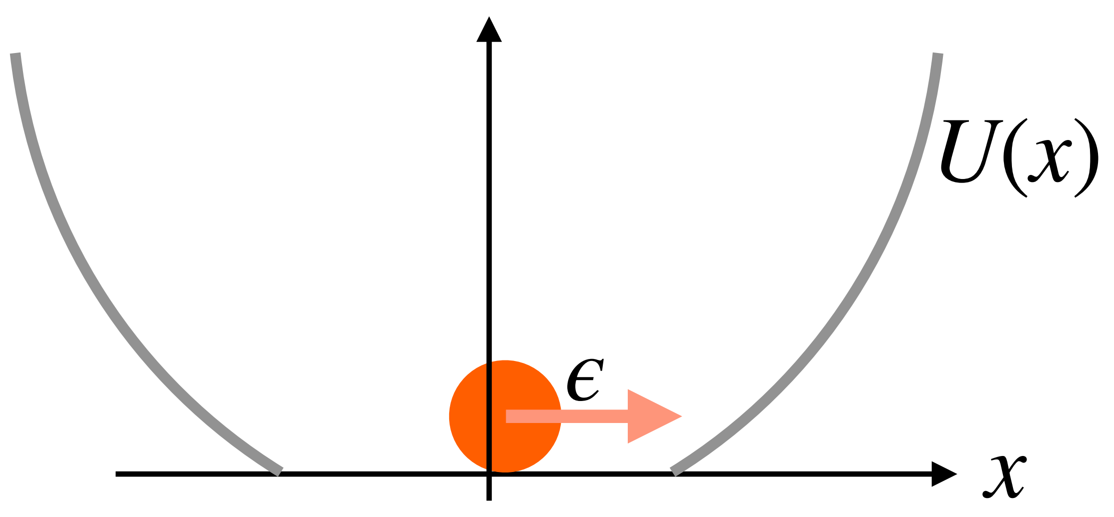
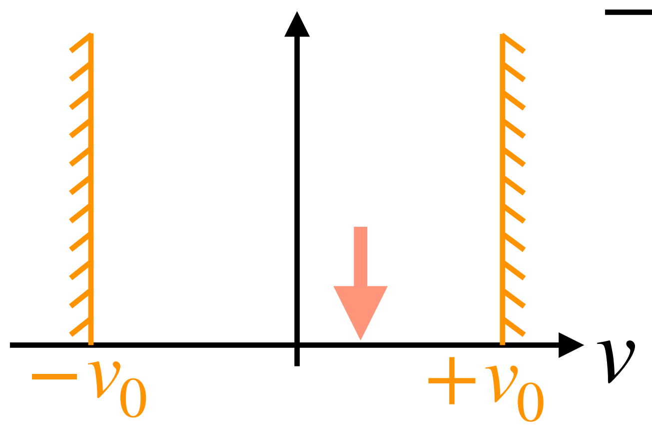
Correct active dynamics, but NO interactions.





Continuous-time limit

How do we also capture the confining potential?

$$v = \frac{\epsilon}{dt} \quad t = ndt \quad \langle \Delta v^2(t) \rangle = \sqrt{2D_v t}$$

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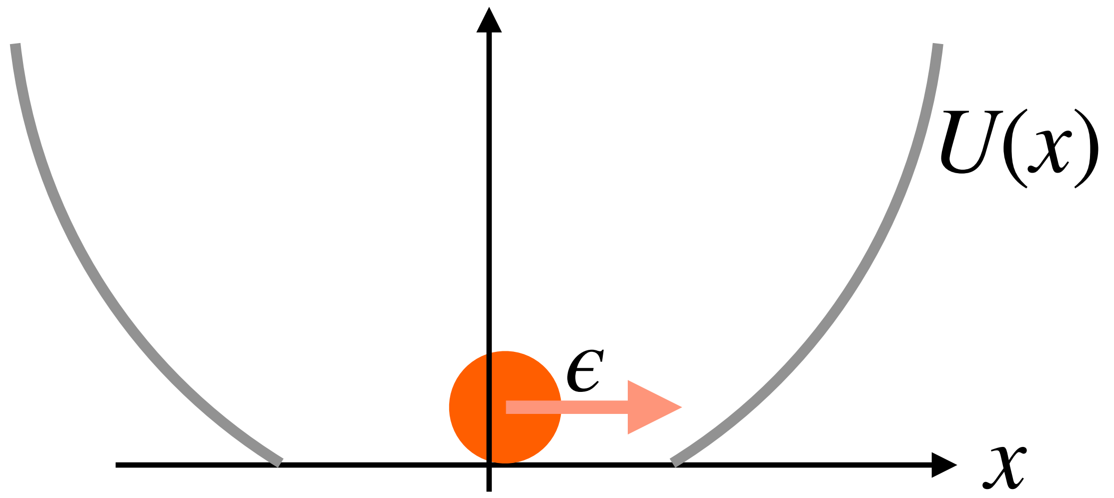

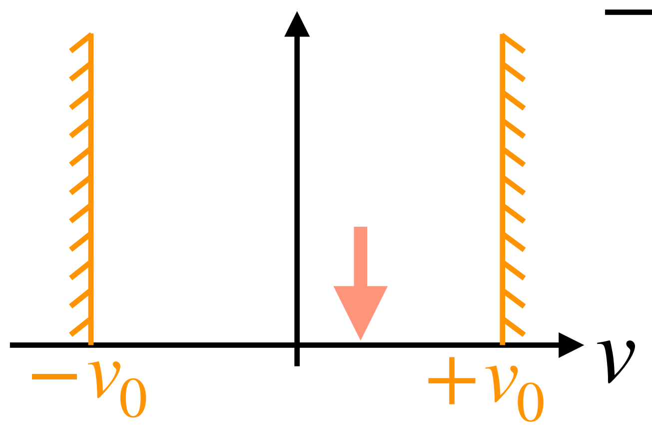

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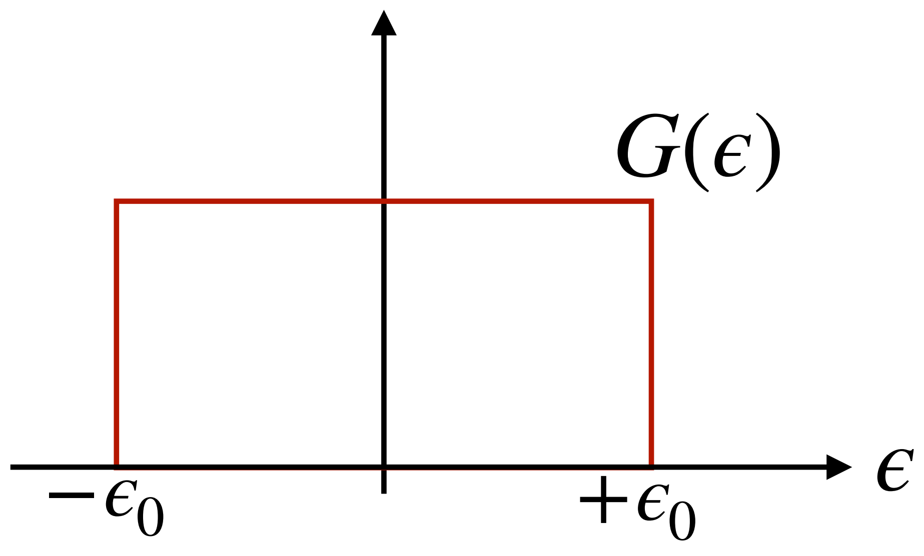

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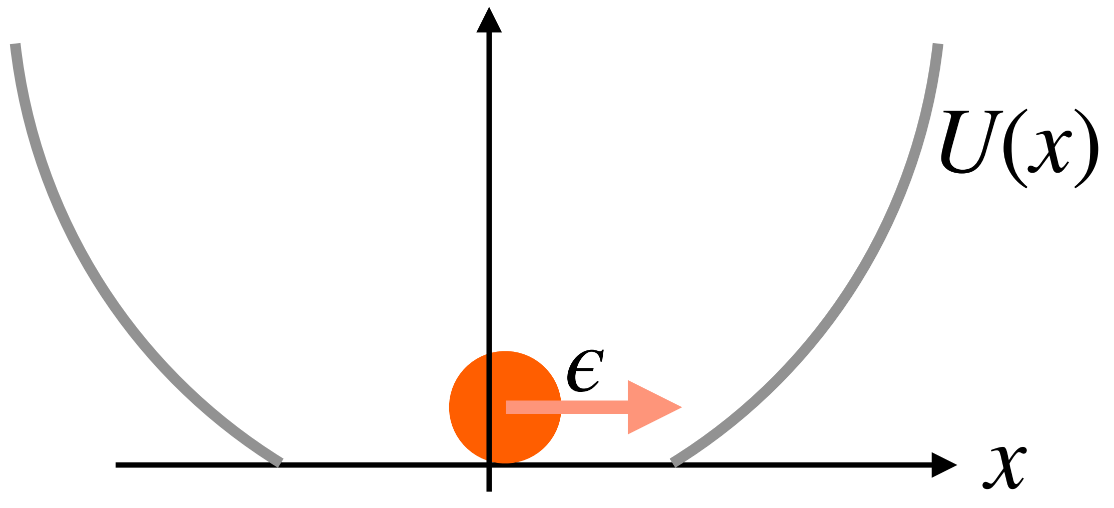
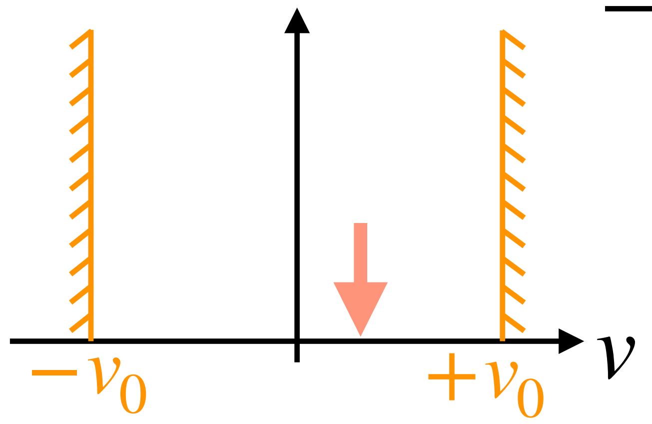
Continuous-time limit





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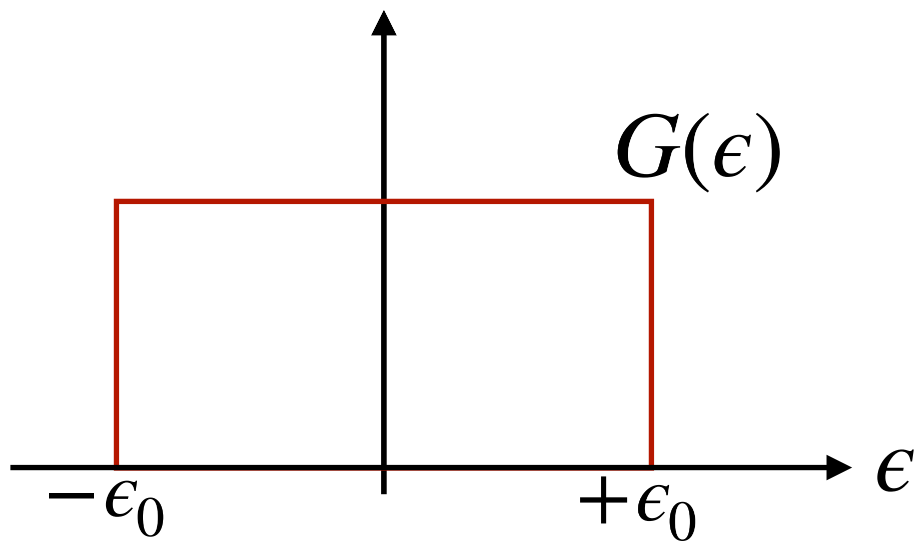

$$\left\langle \Delta \mathbf{r}(t)^2 \right\rangle = \sqrt{2D\, t}$$

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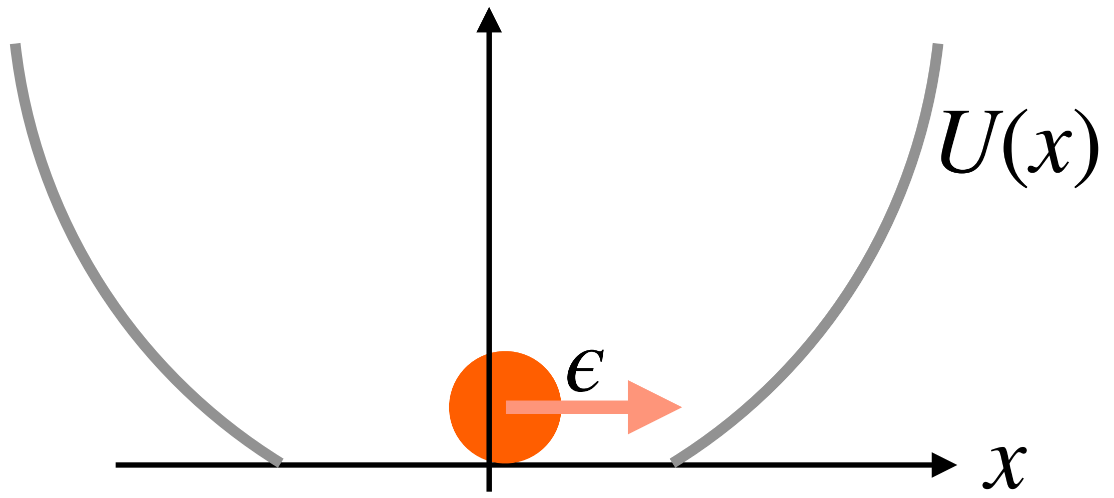

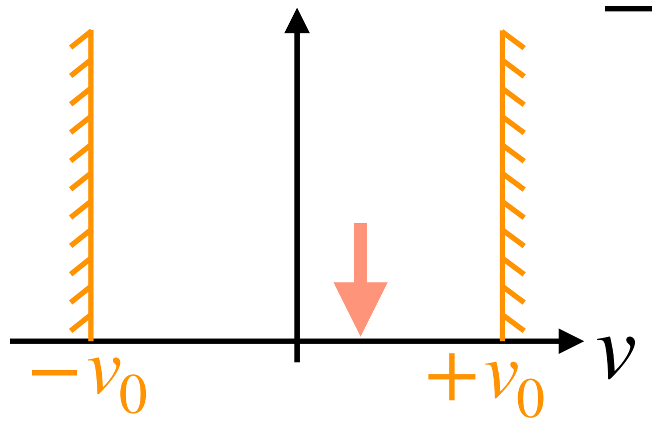

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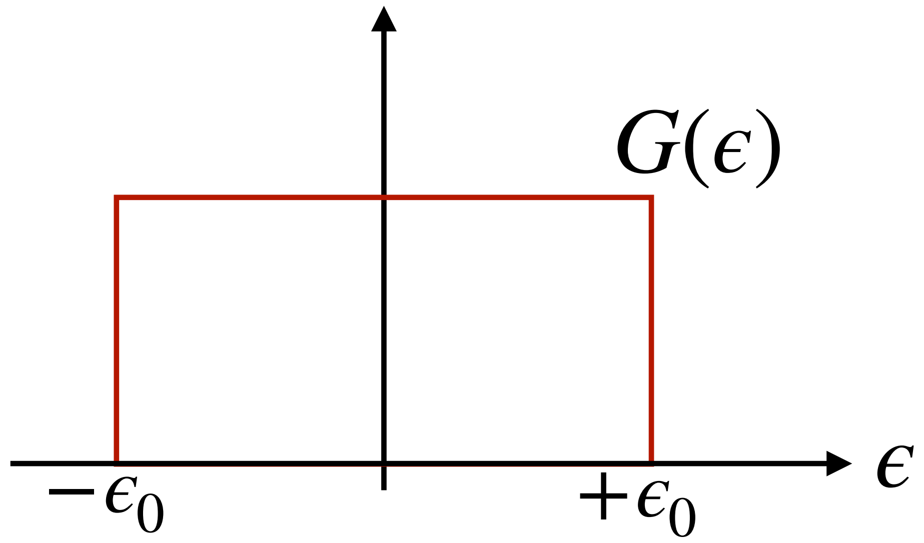

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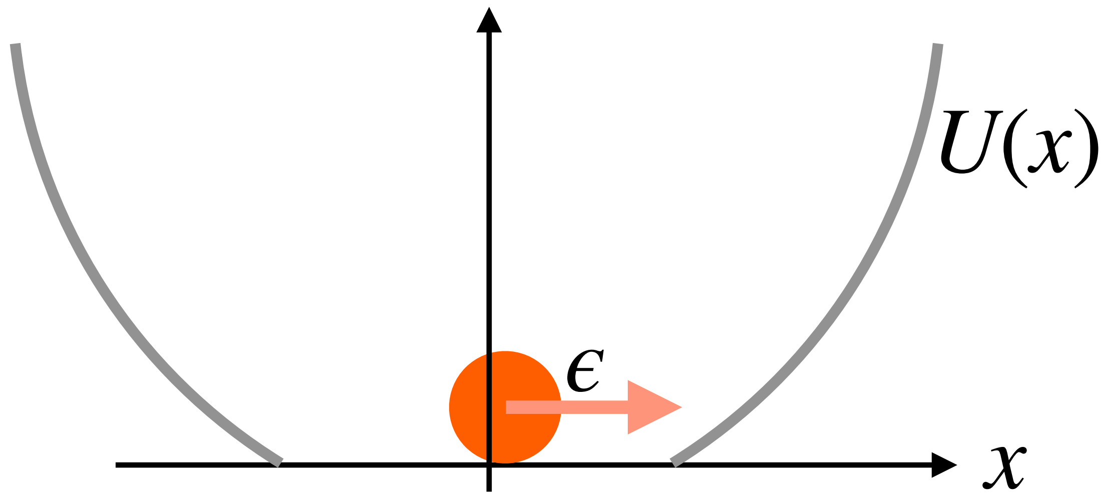

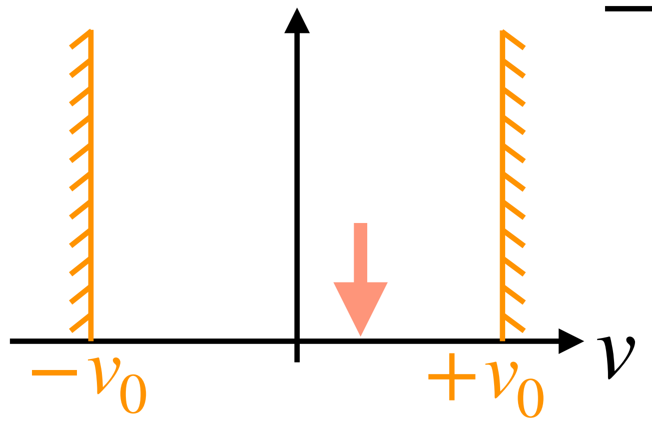

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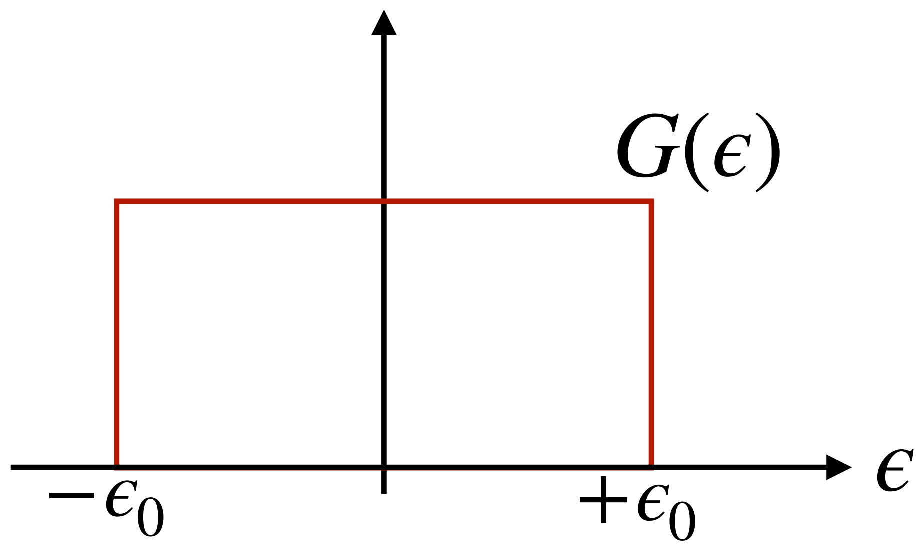

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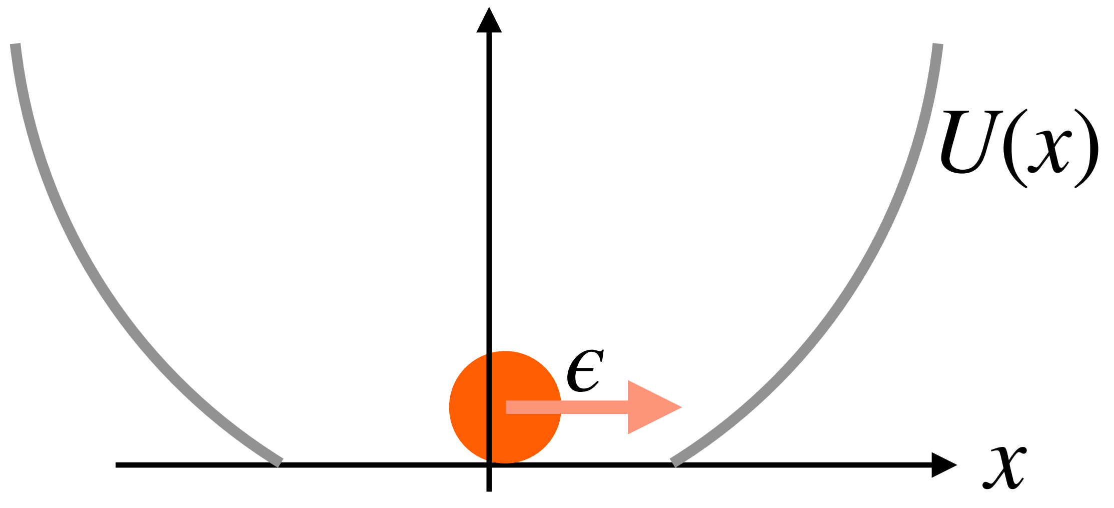
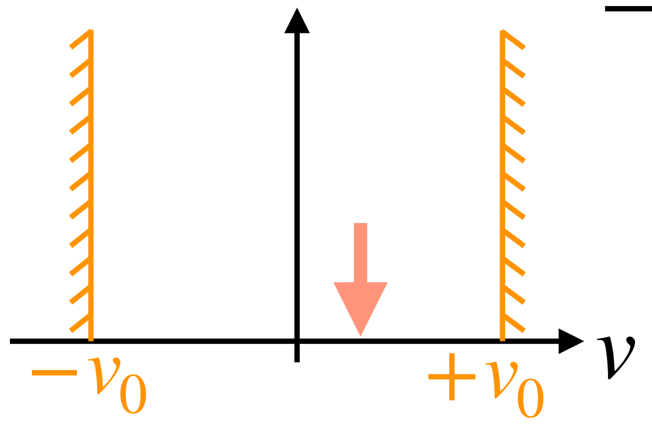
Continuous-time limit





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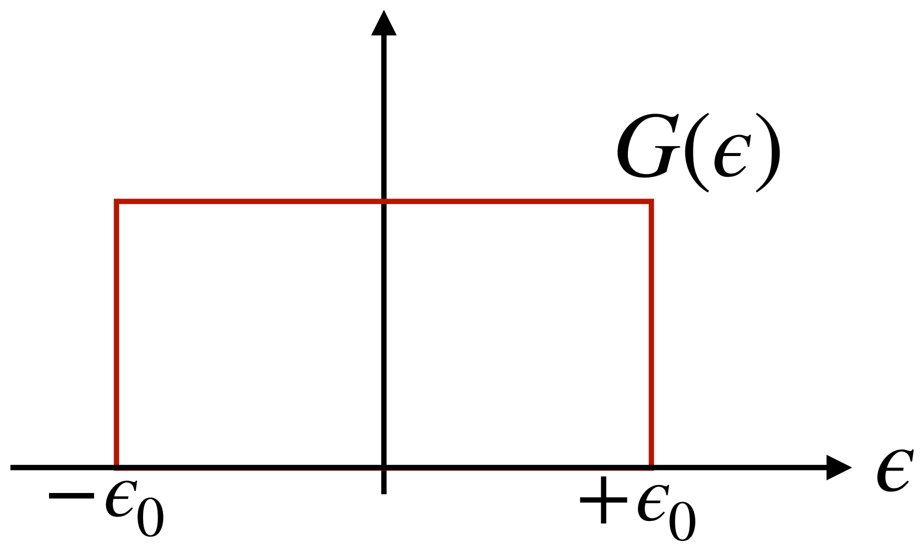

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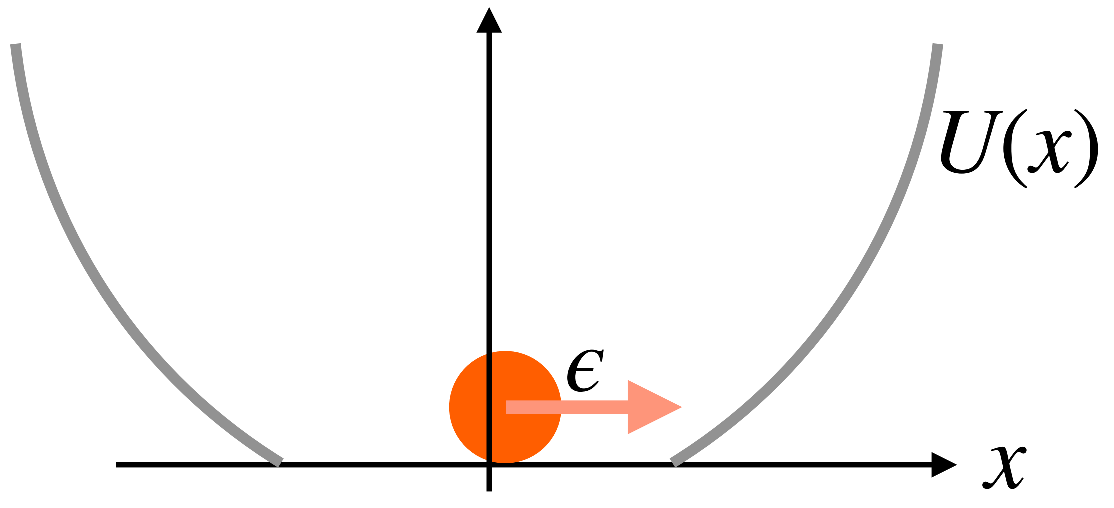
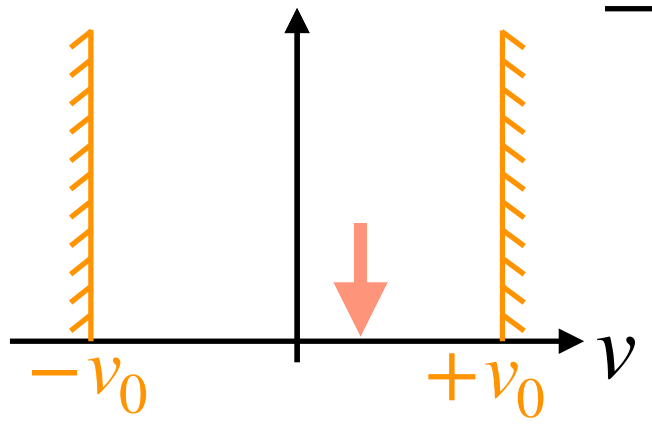
Interactions (and thermal noise).

Continuous-time limit





$$v = \frac{\epsilon}{dt} \quad t = ndt \quad \langle \Delta v^2(t) \rangle = \sqrt{2D_v t}$$

$$dt \to 0 \quad \text{with} \quad v_0 = \text{const}, \quad \tau = \text{const}$$

$$P_{n+1}(x, v) = \int_{-\infty}^{+\infty} dx' \int_{-v_0}^{v_0} dv'\, g\left(v \mid v'\right) W\left(x \mid x', v'dt\right) P_n(x', v')$$

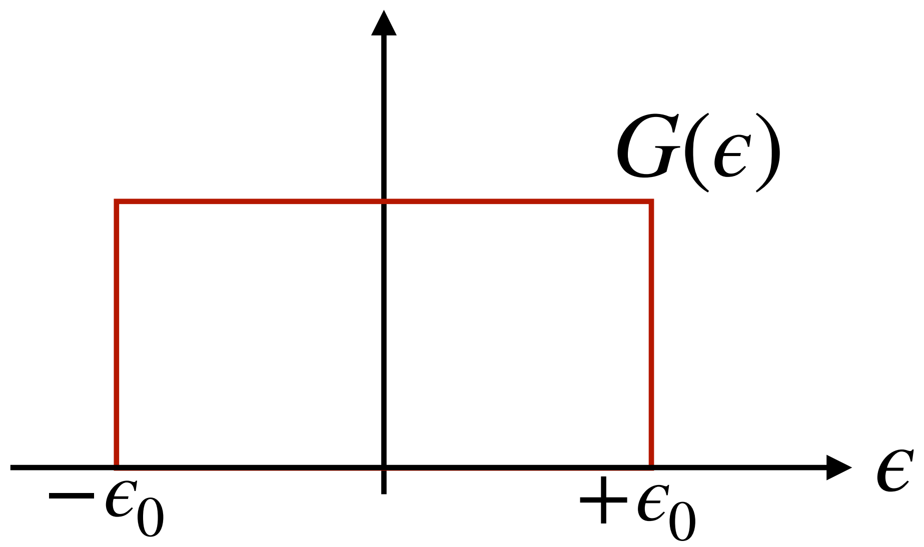
Kramers-Moyal expansion

$$\frac{\partial P_t(x, v)}{\partial t} = D_v \frac{\partial^2}{\partial v^2} P_t(x, v) - \frac{\partial}{\partial x} v P_t(x, v)$$

$$\frac{dx}{dt} = v \cancel{-\mu U'(x)} \; ; \; \frac{dv}{dt} = \sqrt{2D_v}\xi(t)$$

Correct active dynamics, but NO interactions.

How do we also capture the confining potential?



$$\left\langle \Delta \mathbf{r}(t)^2 \right\rangle = \sqrt{2D\,t}$$

$$P_{n+1}(x) = \int_{-\infty}^{+\infty} dx' \int_{-\epsilon_0}^{\epsilon_0} d\epsilon\, G(\epsilon)\, W\left(x \mid x', \epsilon\right) P_n(x')$$

Kramers-Moyal expansion

$$\frac{\partial P_t(x)}{\partial t} = D \frac{\partial^2}{\partial x^2} P_t(x) - \mu \frac{\partial}{\partial x} U'(x) P_t(x)$$

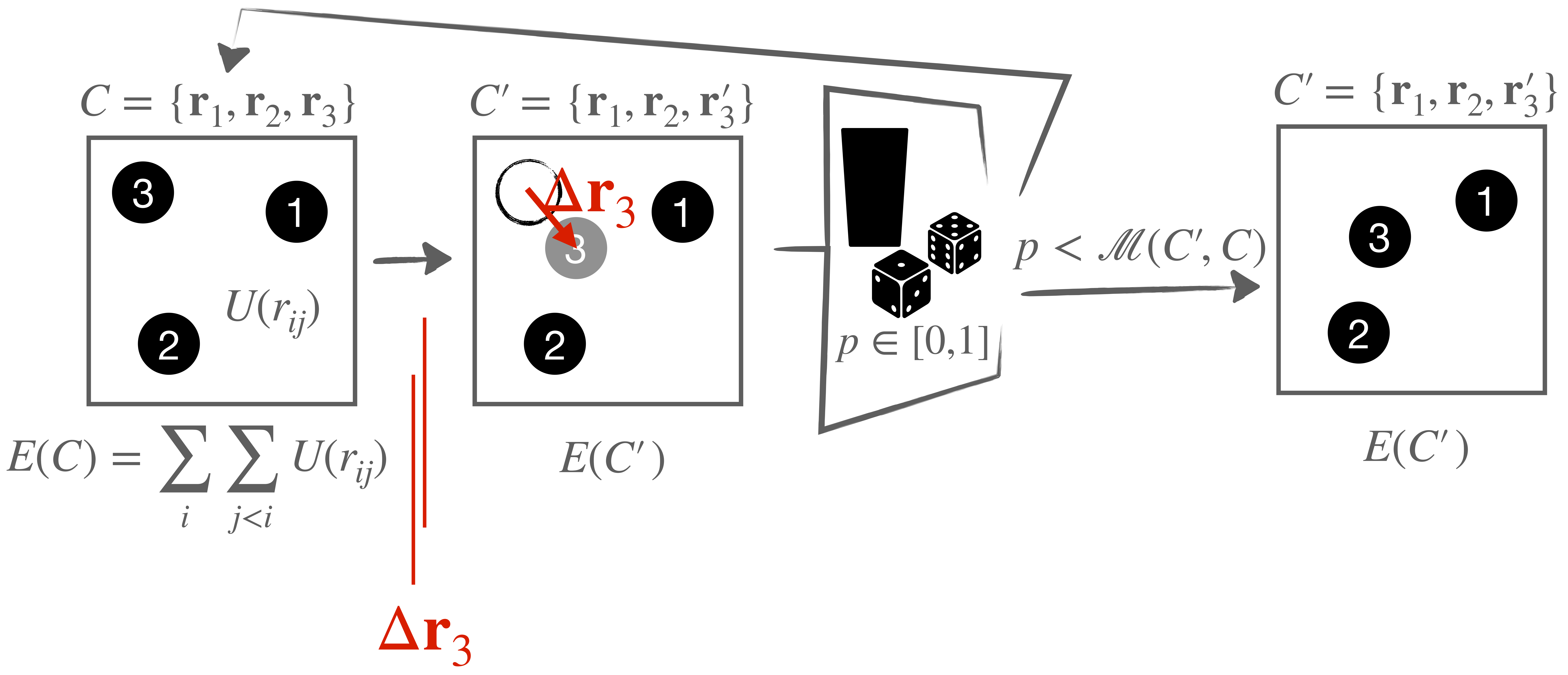
$$\frac{dx}{dt} = -\mu U'(x) + \sqrt{2D}\eta(t)\,, \beta = \mu/D$$

Interactions (and thermal noise).

+

Active Monte Carlo - version 2.0

$$\mathscr{M}(C', C) = \min\left\{1, e^{-\beta[E(C')-E(C)]}\right\}$$



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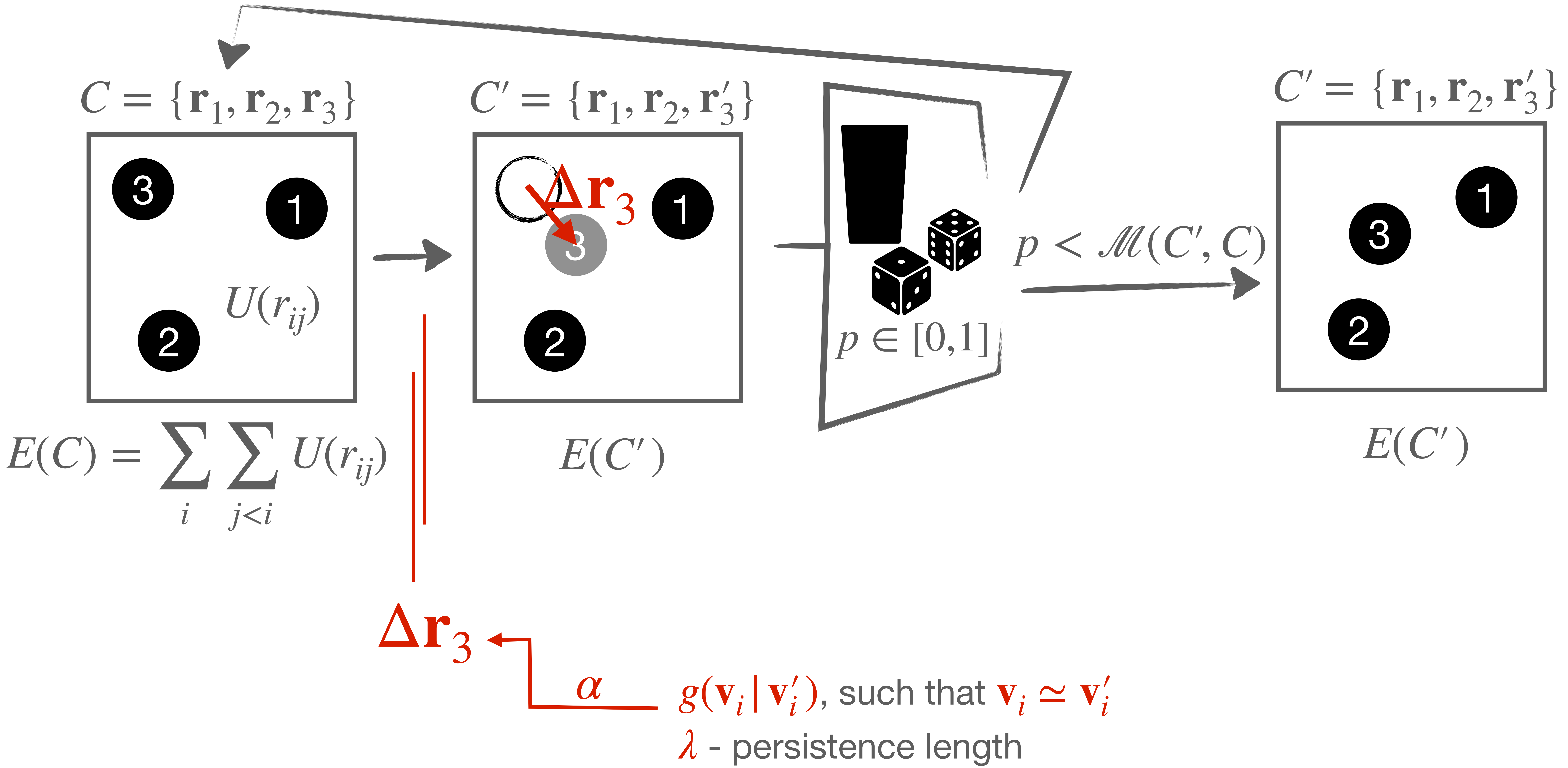

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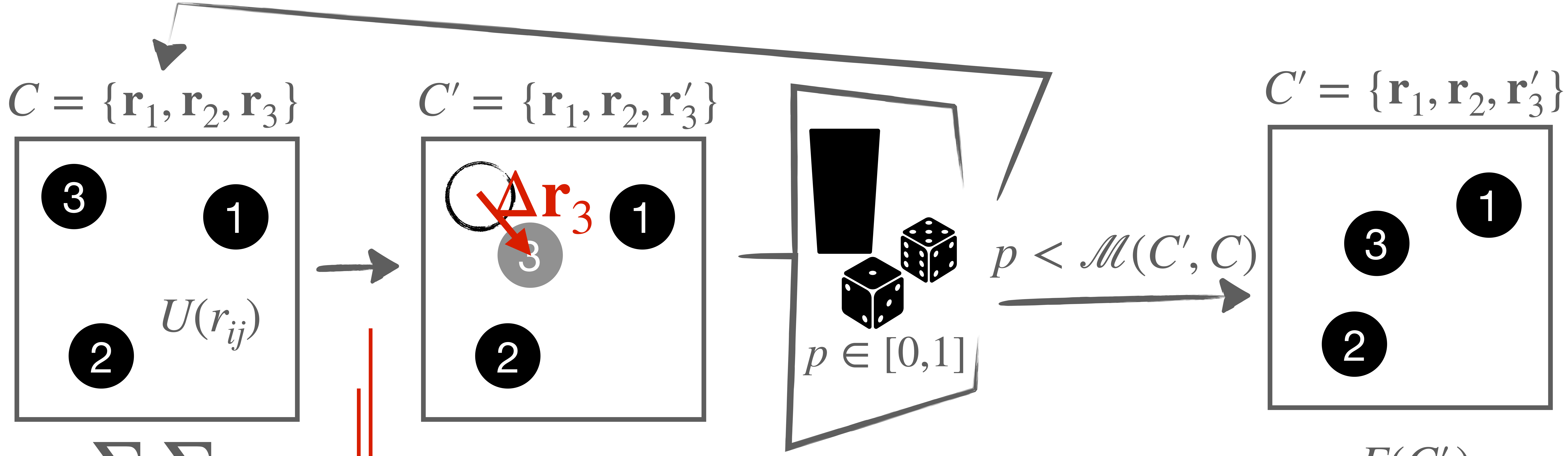


$$E(C) = \sum_i \sum_{j<i} U(r_{ij})$$

$E(C')$

$E(C')$

$\Delta\mathbf{r}_3$

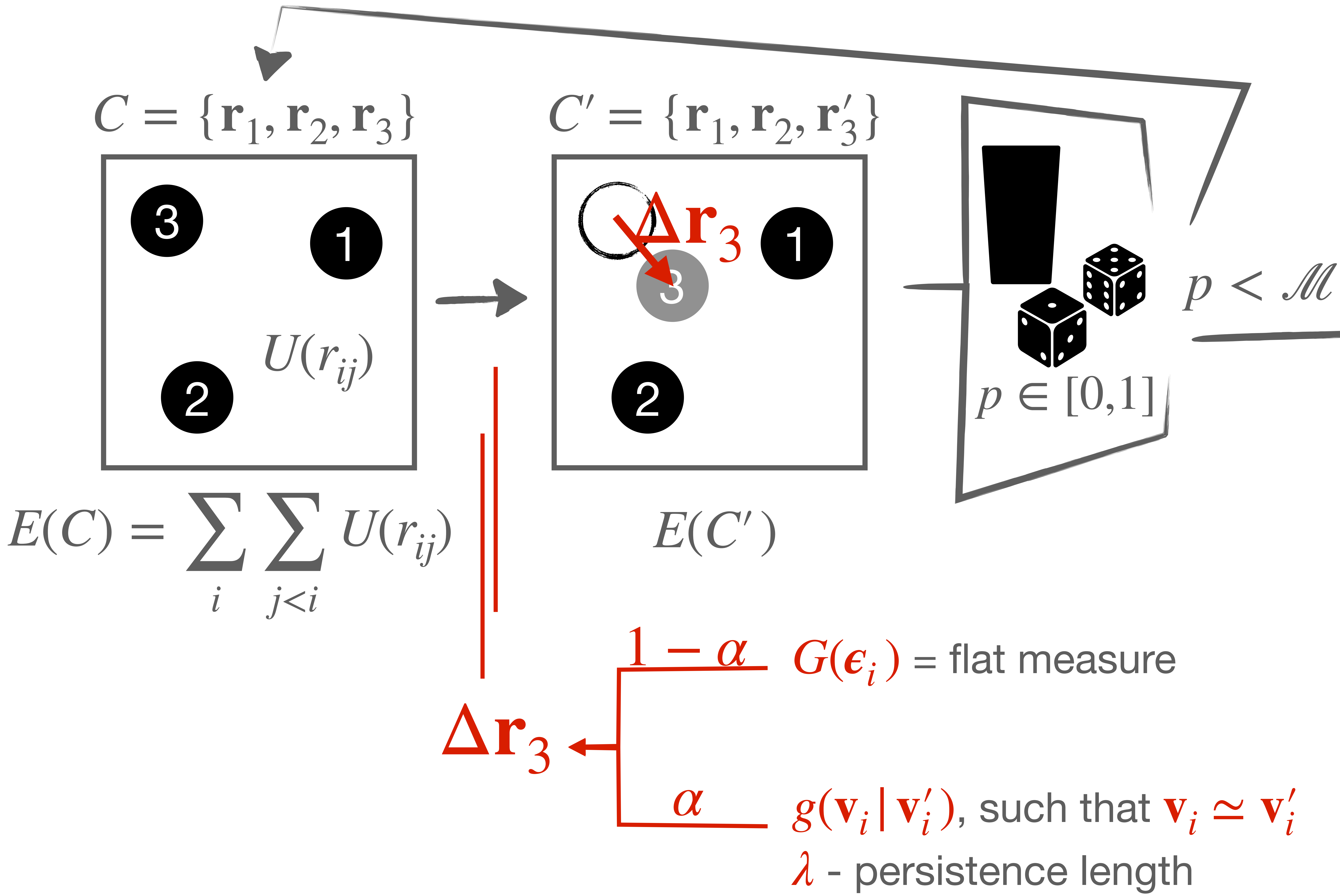
$1-\alpha$: $G(\epsilon_i)$ = flat measure

α: $g(\mathbf{v}_i \,|\, \mathbf{v}'_i)$, such that $\mathbf{v}_i \simeq \mathbf{v}'_i$

λ - persistence length

Active Monte Carlo - version 2.0

$$\mathscr{M}(C', C) = \min\left\{1, e^{-\beta[E(C') - E(C)]}\right\}$$



Test EQUIVALENCE with Langevin models !?

How to test?

$$\frac{d\boldsymbol{r}_i}{dt} = \mathbf{v}_i(t) + \mu \sum_{j \neq i} \boldsymbol{F}(\boldsymbol{r}_{ij}) + \sqrt{2D}\, \boldsymbol{\eta}_i(t)$$

How to test?

$$\frac{d\boldsymbol{r}_i}{dt} = \mathbf{v}_i(t) + \mu \sum_{j \neq i} \boldsymbol{F}(\boldsymbol{r}_{ij}) + \sqrt{2D}\,\boldsymbol{\eta}_i(t)$$

Active Brownian Particles

$$\mathbf{v}_i = v_0 \mathbf{n}(\theta_i)\,; \quad \frac{d\theta_i}{dt} = \sqrt{2D_r}\xi_i$$

Active Ornstein-Uhlenbeck Process

$$\tau \frac{d\mathbf{v}_i}{dt} = -\mathbf{v}_i + \sqrt{2D_v}\boldsymbol{\xi}_i$$

Run-And-Tumble Particles

$$\mathbf{v}_i = v_0 \mathbf{n}(\theta_i)$$

θ_i sampled uniformly at finite rate

Active Random-Acceleration Process

$$\frac{d\mathbf{v}_i}{dt} = \sqrt{2D_v}\xi_i$$

& reflecting boundaries at $|\mathbf{v}| = v_0$

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Thermodynamic pressure:

$$\mathscr{P}_{ideal} = \rho_{\mathrm{bulk}}\,(k_{\mathrm{B}}T + \mathrm{const})$$

A. P. Solon et al Nature Phys (2015).

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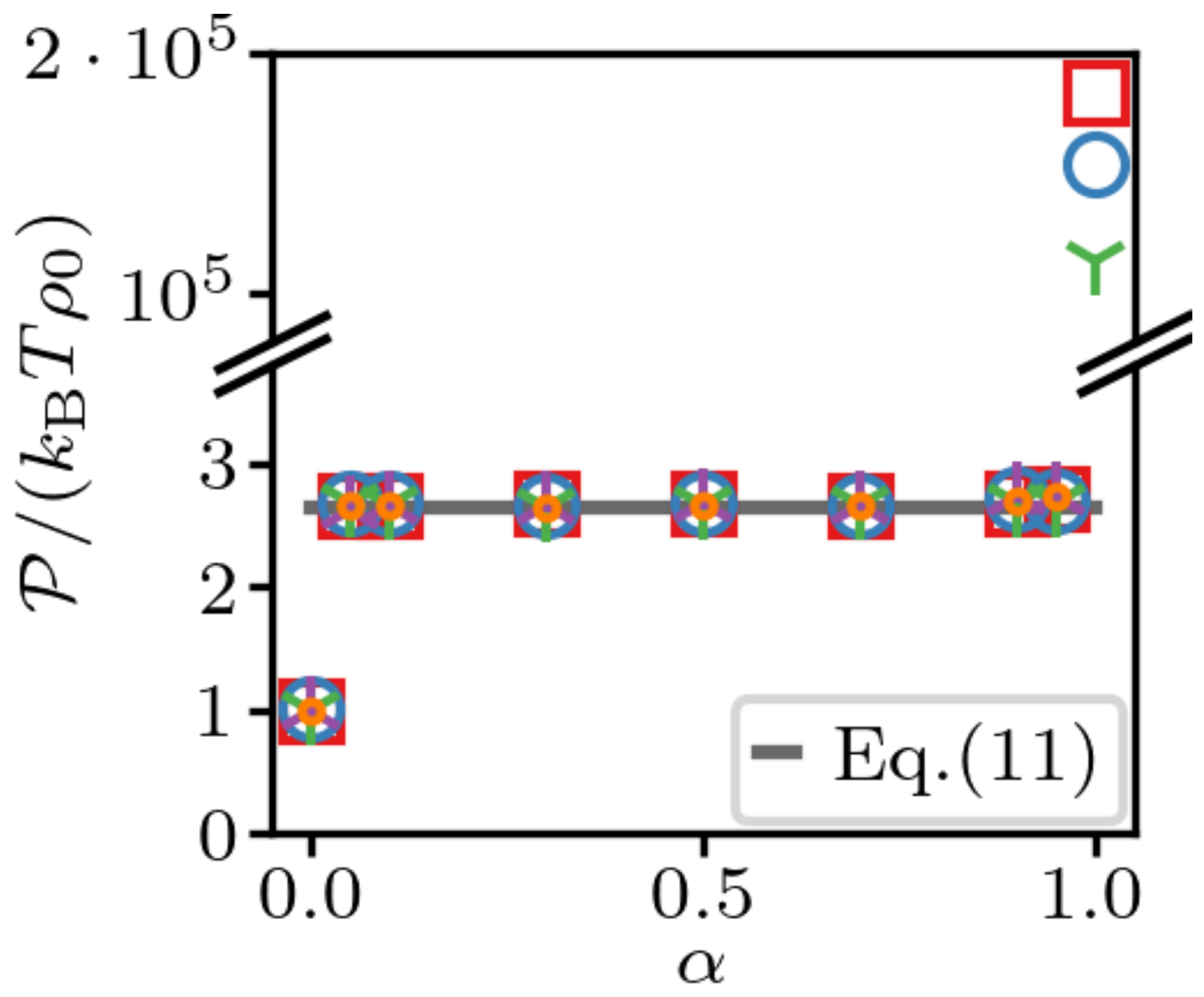
$$P_{n+1}(\mathbf{r},\mathbf{v}) = \int d\mathbf{r}' \int d\mathbf{v}'\, M(\mathbf{r},\mathbf{v}\,|\,\mathbf{r}',\mathbf{v}')P_n(\mathbf{r}',\mathbf{v}')$$

$$M(\mathbf{r},\mathbf{v}\,|\,\mathbf{r}',\mathbf{v}') = g(\mathbf{v}\,|\,\mathbf{v}')\left[\alpha\, W(\mathbf{r}\,|\,\mathbf{r}',\mathbf{v}'dt) + (1-\alpha)\int G(\epsilon)W(\mathbf{r}\,|\,\mathbf{r}',\epsilon)\right]$$



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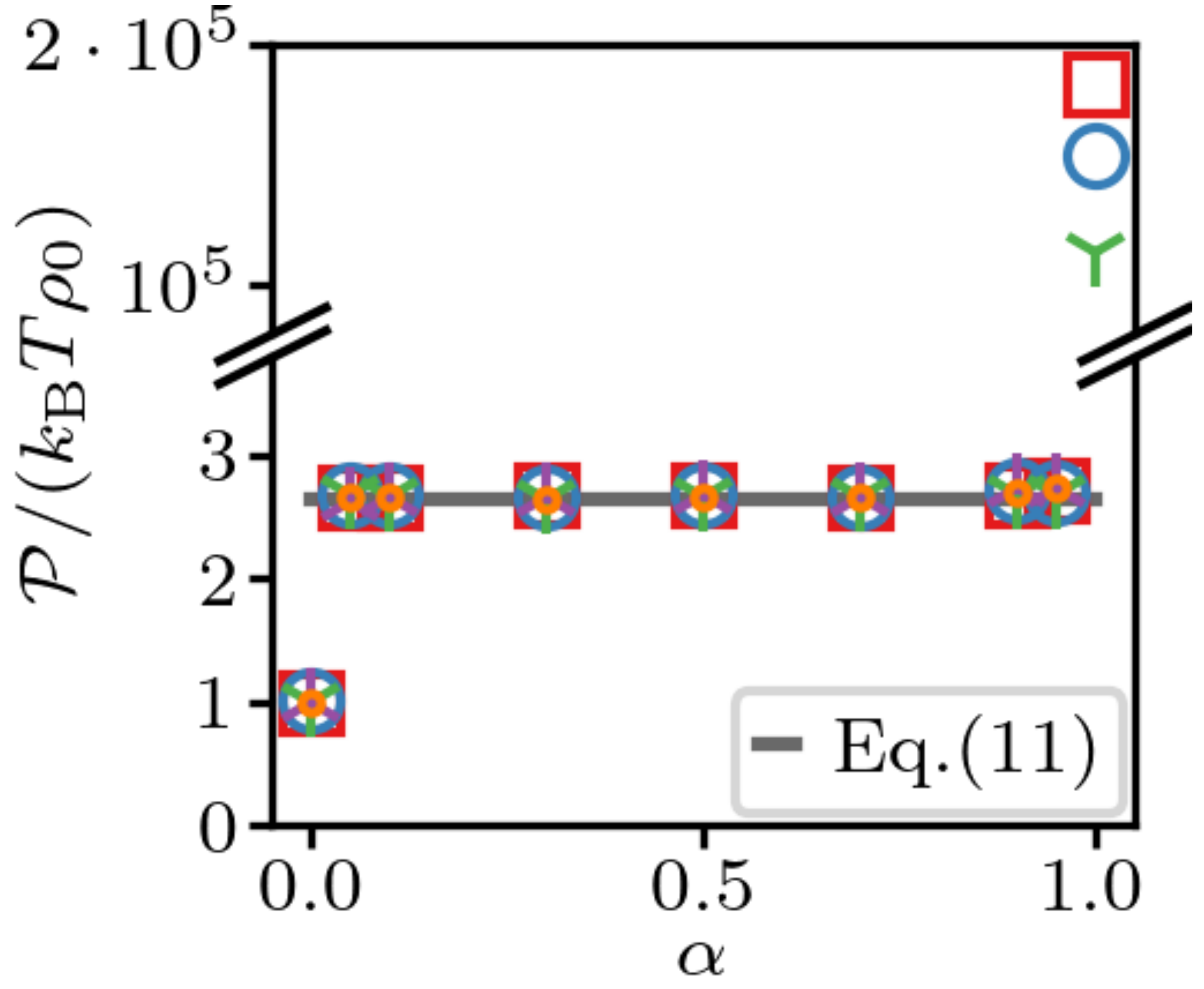
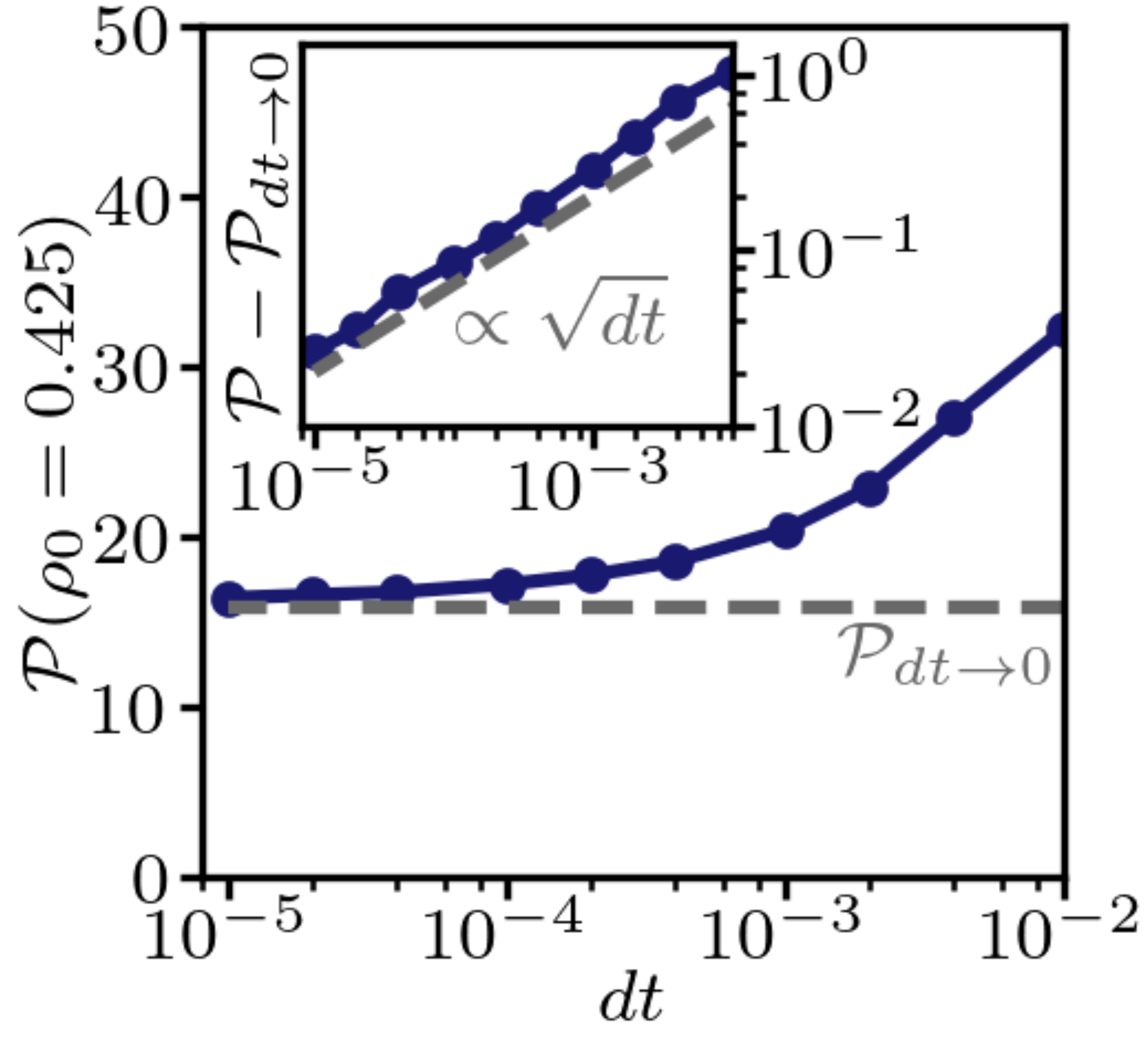


$dt \to 0$



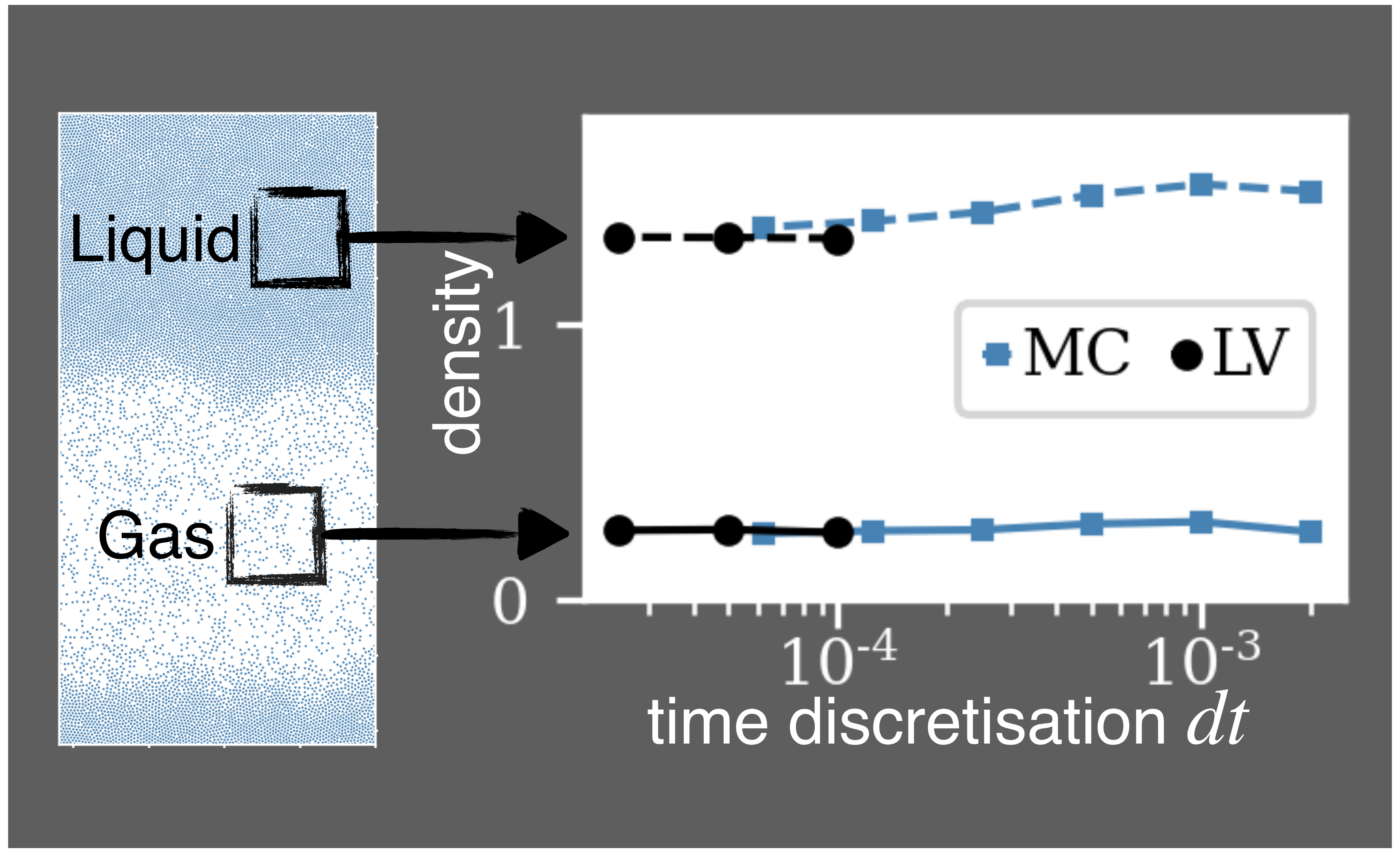
Conclusion

Collective behaviour of persistent particles with active Monte Carlo

- D. Levis, L. Berthier, Phys. Rev. E (2014).
- L. Berthier, Phys Rev Lett (2014).
- **J. Klamser**, S. Kapfer, W. Krauth, Nat Commun (2018).
- **J. Klamser**, S. Kapfer, W. Krauth, J Chem Phys (2019).

Connection to standard models via continuous-time limit

Kinetic Monte Carlo Algorithms for Active Matter Systems
Juliane U. Klamser, Olivier Dauchot, Julien Tailleur
Phys. Rev. Lett. **127** (2021), 150602



Other MC approaches

Kinetic Event-Chain Algorithm for Active Matte
T. A. Kampmann, T. Sathiyanesan and J. Kierfeld
arXiv (2021)