Simulating the standard active-matter models with Monte Carlo methods

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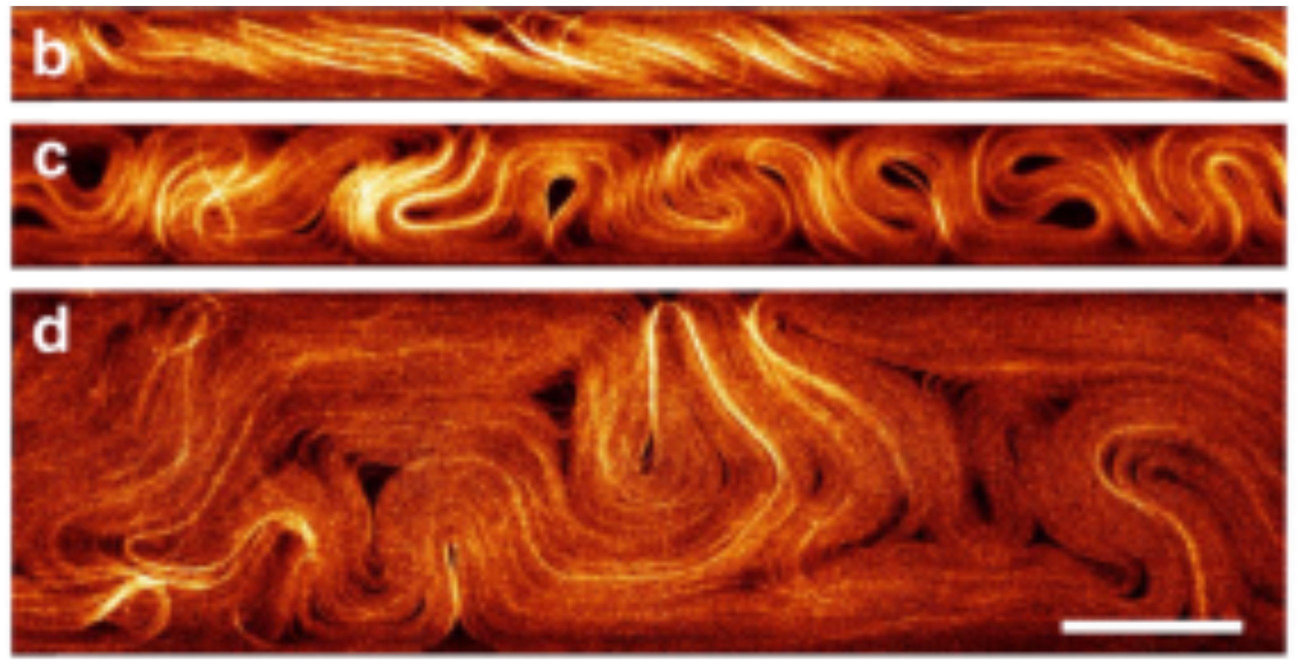
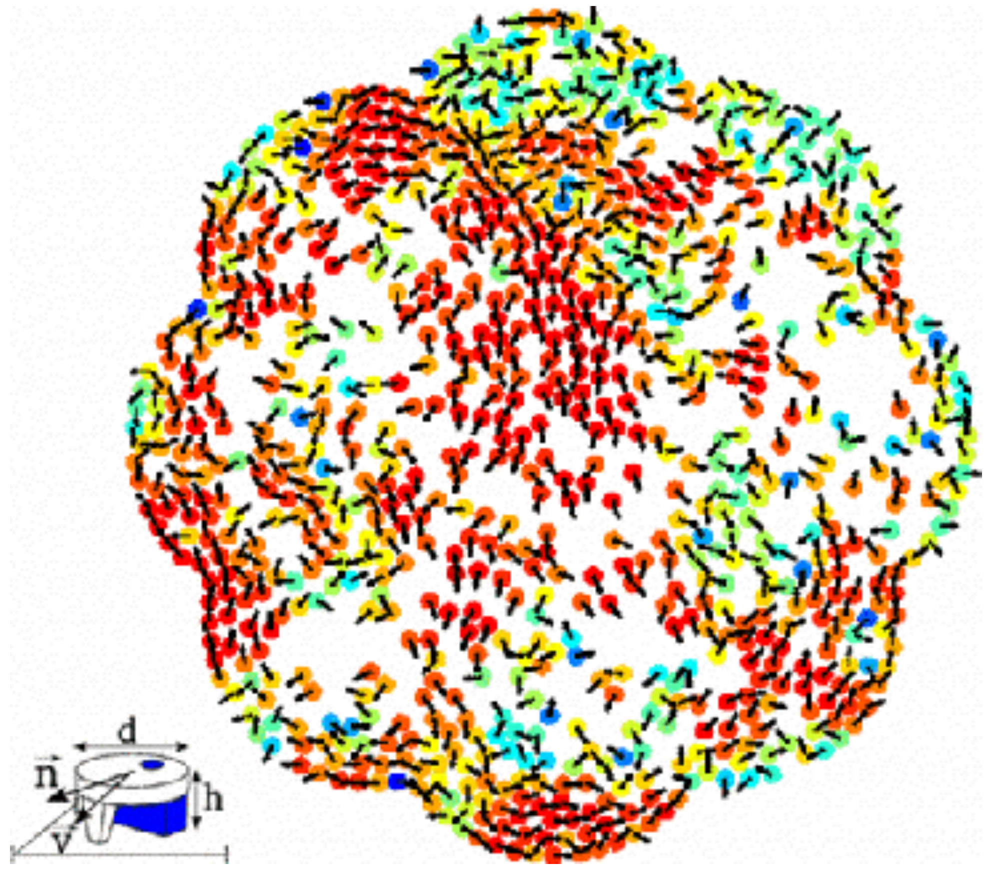
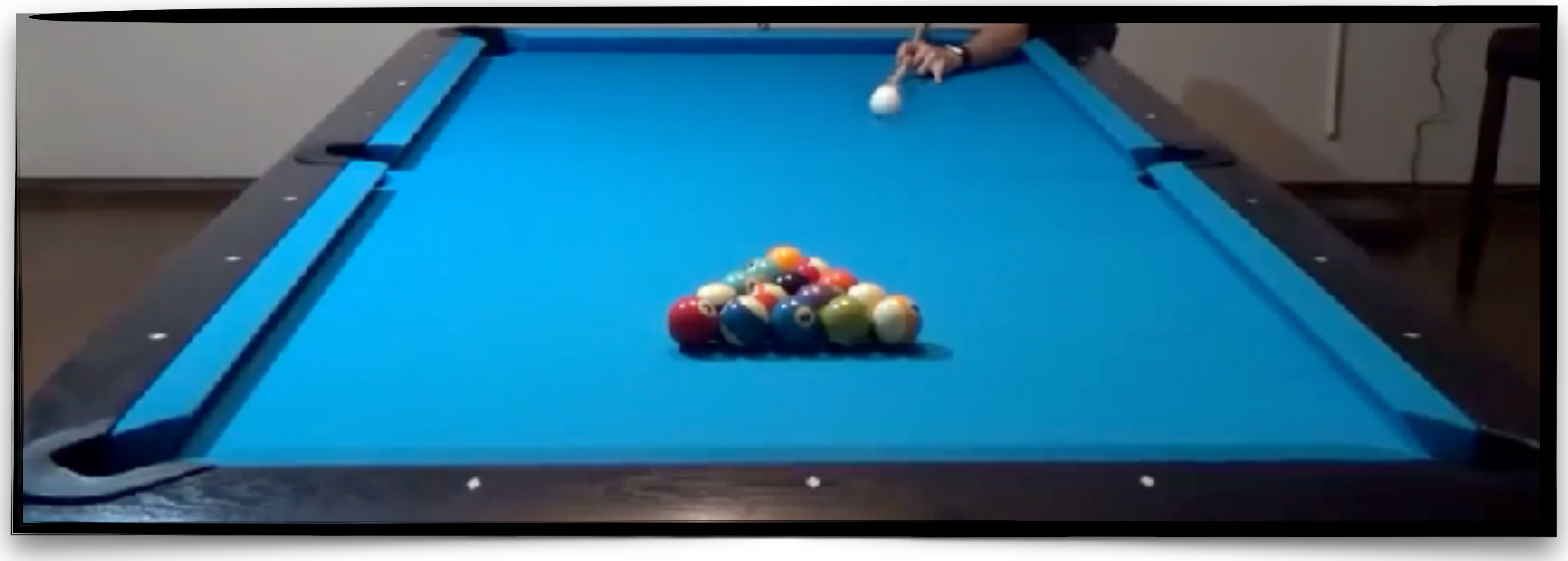
Experimental Active matter:





Hardoüin, J., Hughes, R., Doostmohammadi, A. *et al.* *Commun Phys* **2,** 121 (2019).

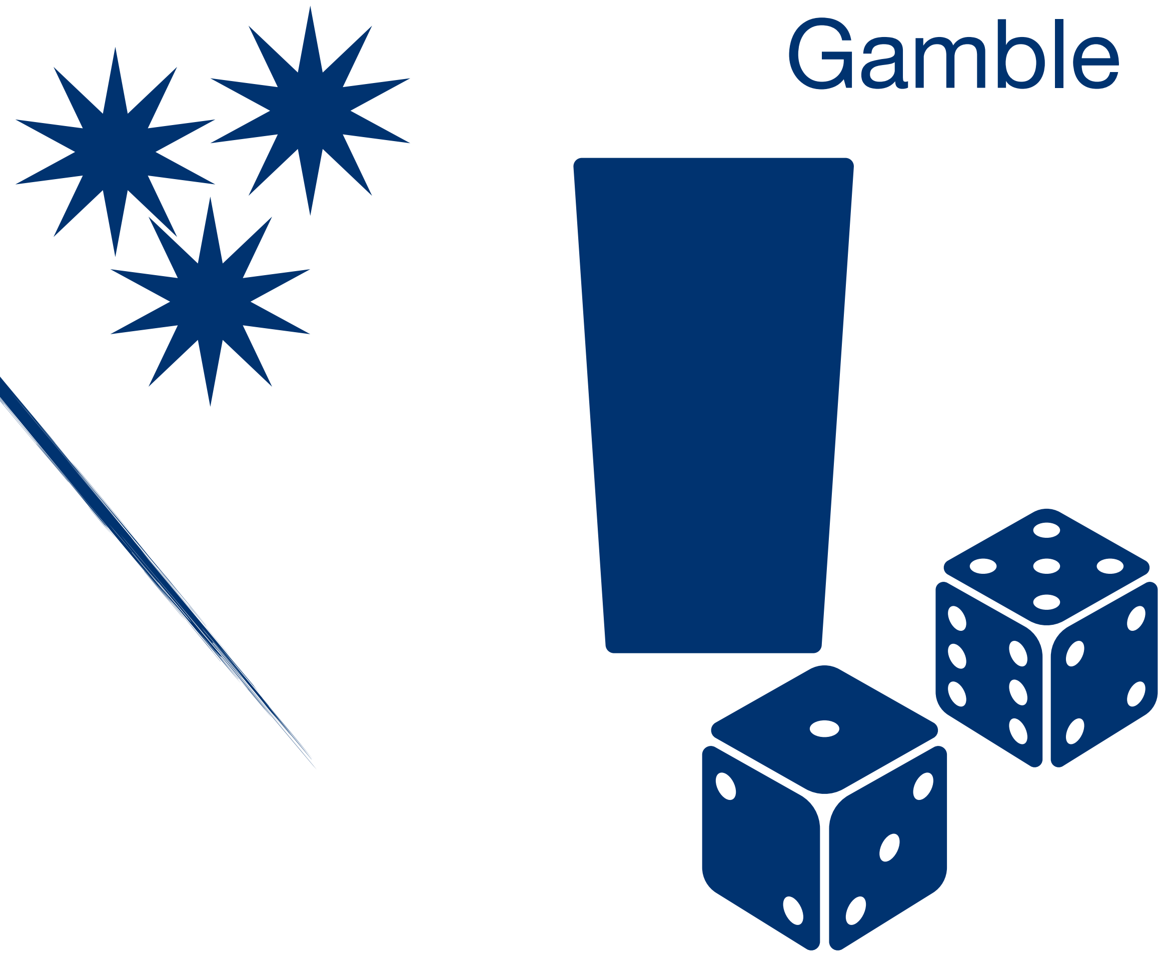
Julien Deseigne, Olivier Dauchot, and Hugues Chaté, Phys. Rev. Lett. **105**, 098001 (2010).



Follow equation of motion

Numerics in equilibrium:

Gamble



Analytical and numerical Active Matter:

Paul Langevin

Active Brownian Particles

$$\dot{\boldsymbol{r}}_i = v_0 \boldsymbol{u}\left(\theta_i\right) + \sum_{j \neq i} \boldsymbol{F}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right) + \sqrt{2D_{\mathrm{t}}}\boldsymbol{\eta}_i$$

$$\dot{\theta}_i = \sqrt{2D_r}\xi_i$$

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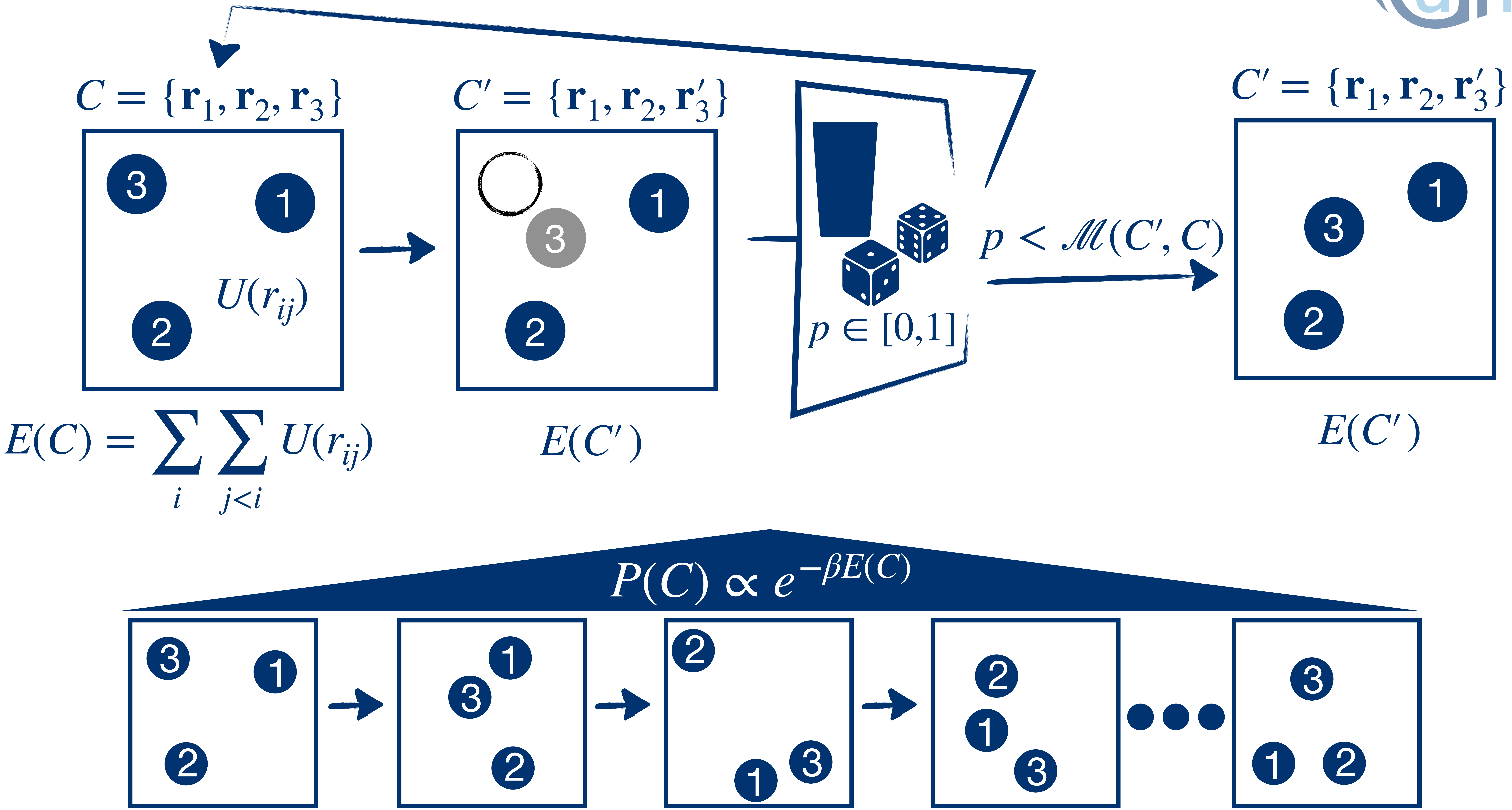
Equilibrium Monte Carlo

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



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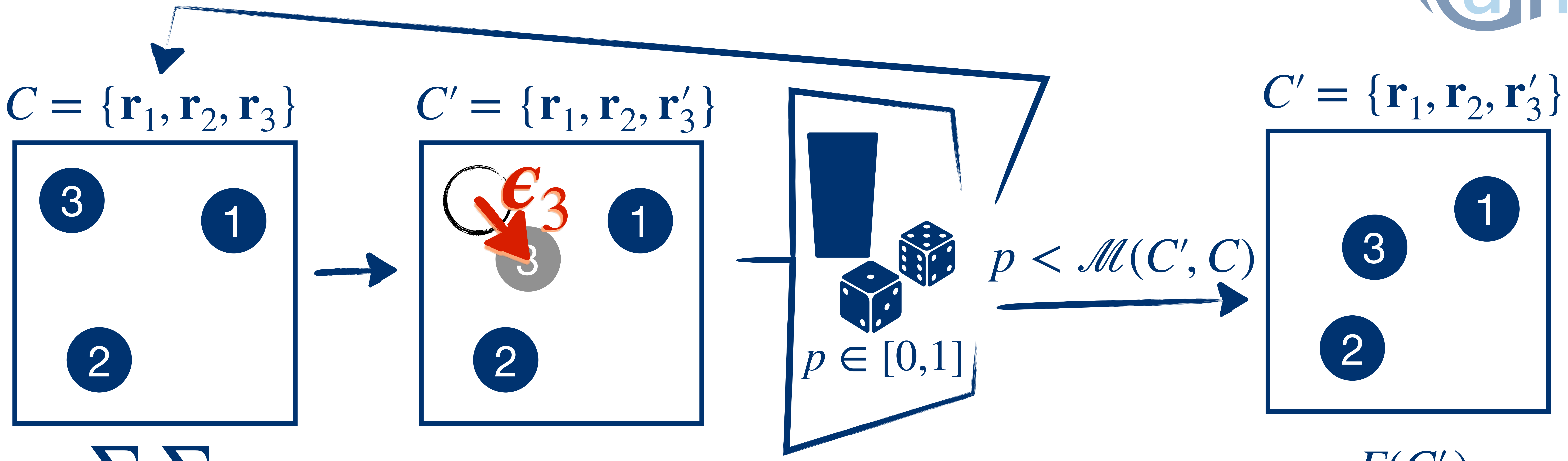
Active Monte Carlo

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



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

$E(C')$

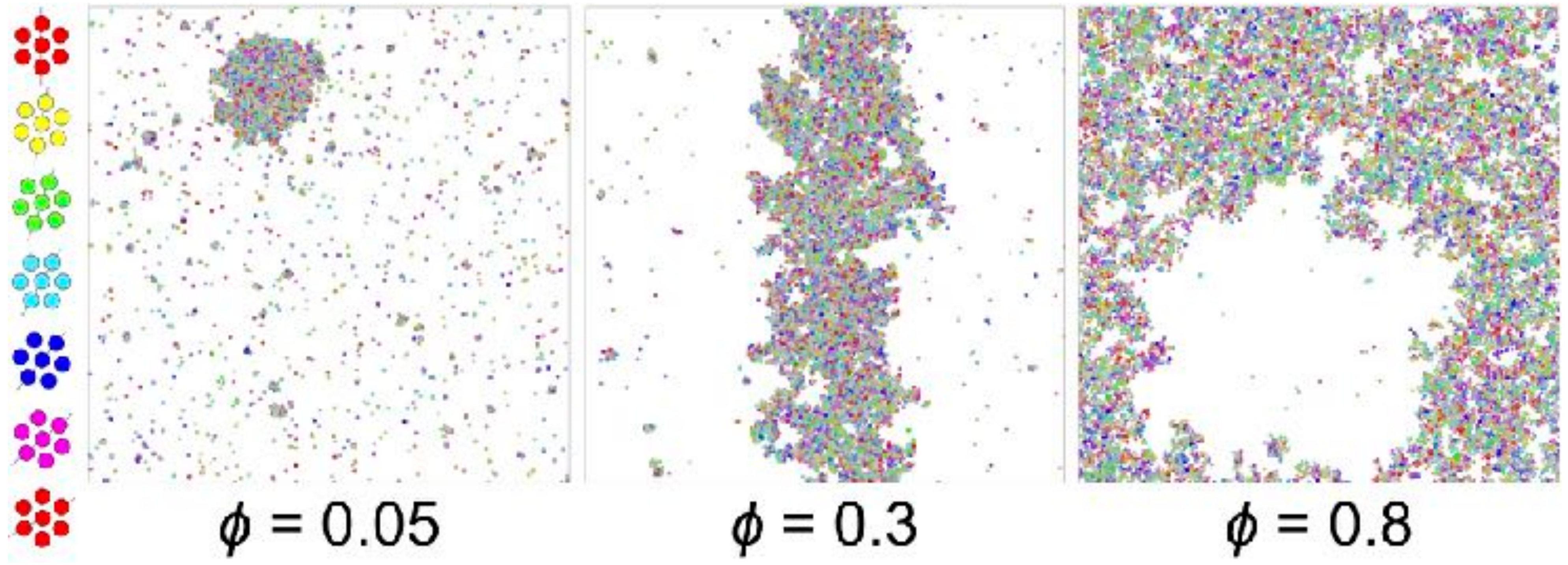
$E(C')$

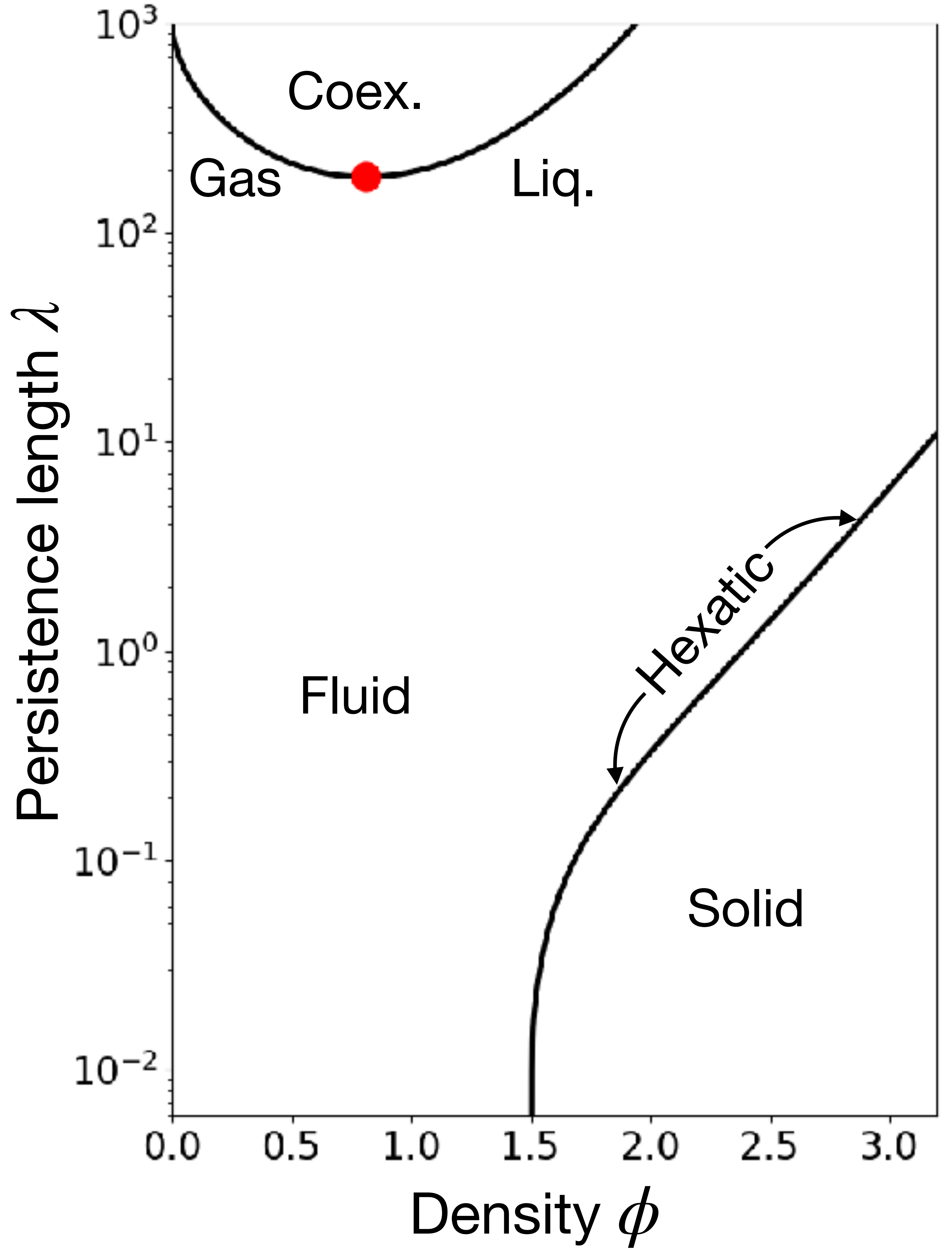
Equilibrium Monte Carlo: $G(\epsilon_i)$ = flat measure

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

λ - persistence length

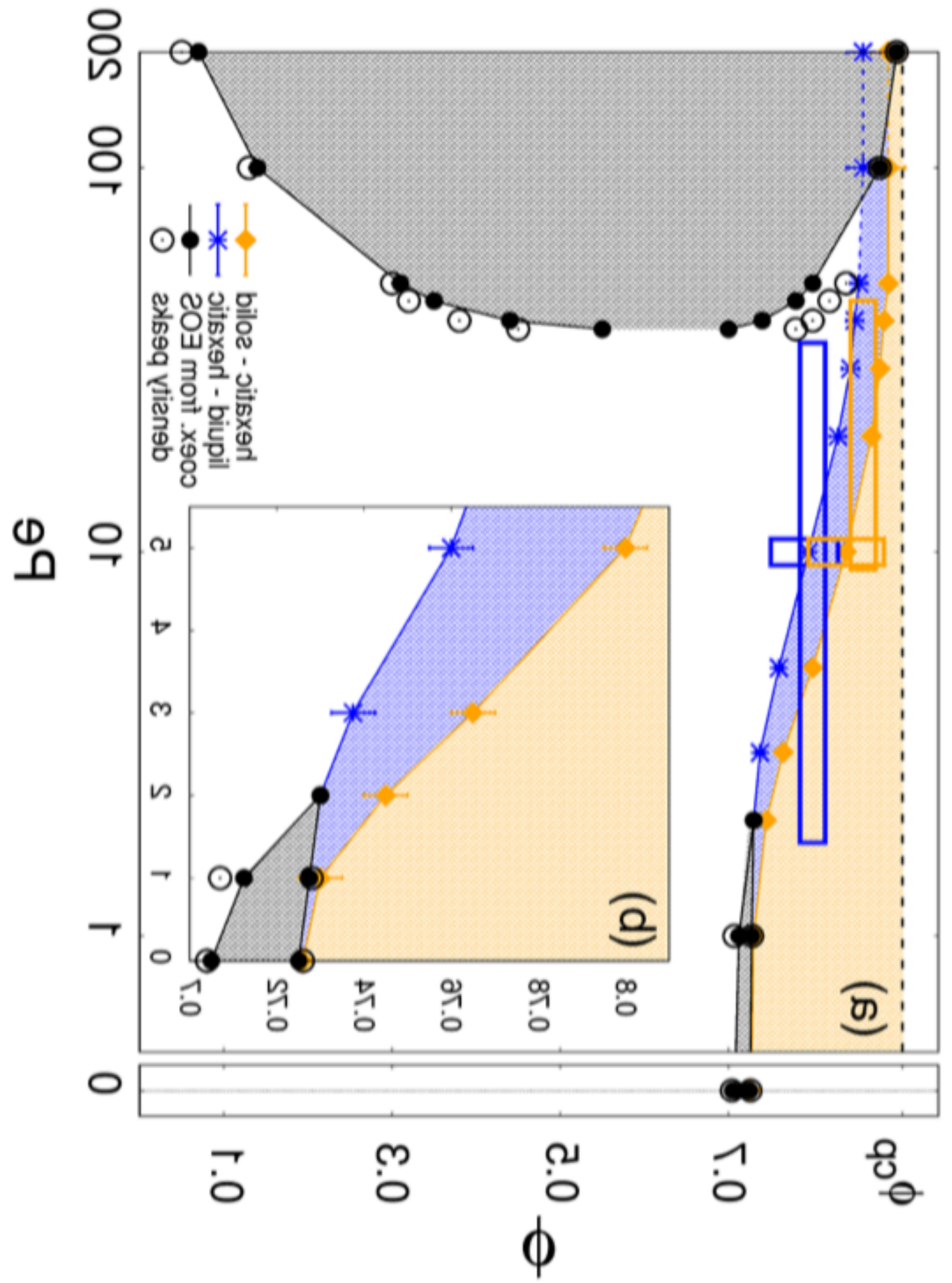
- D. Levis, L. Berthier, *Phys. Rev. E* **89**, 062301 (2014).



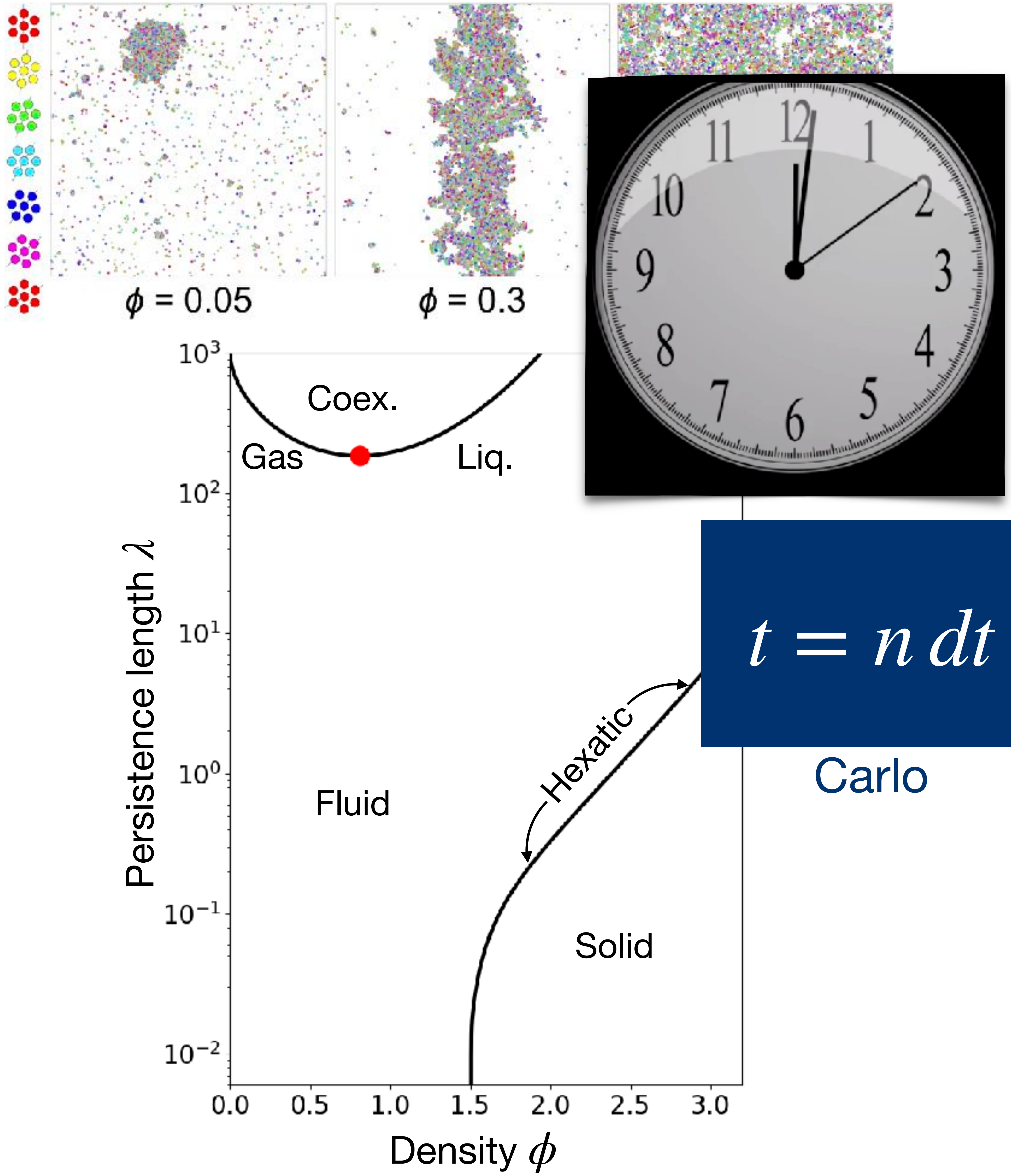


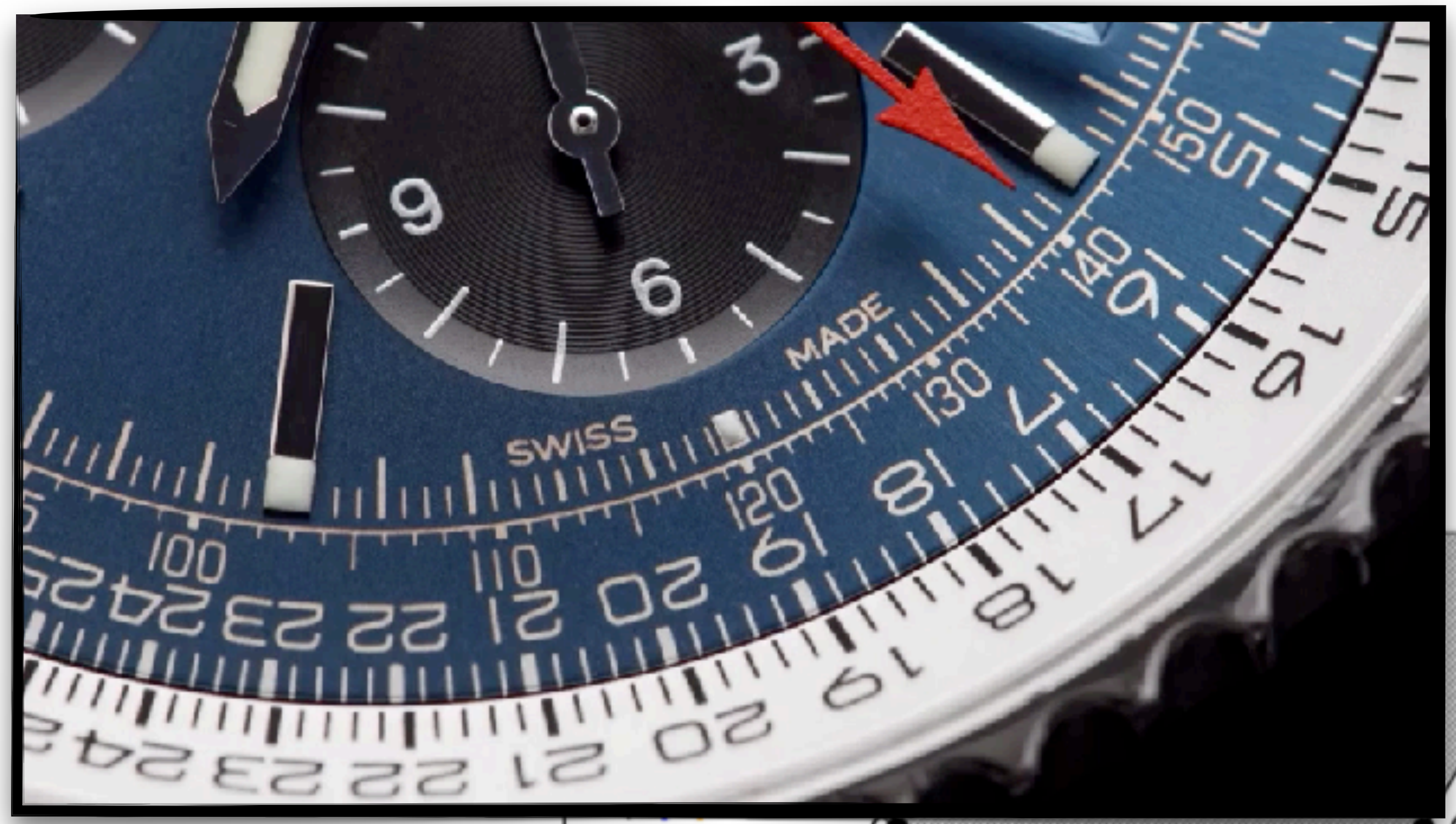
Active Kinetic Monte Carlo

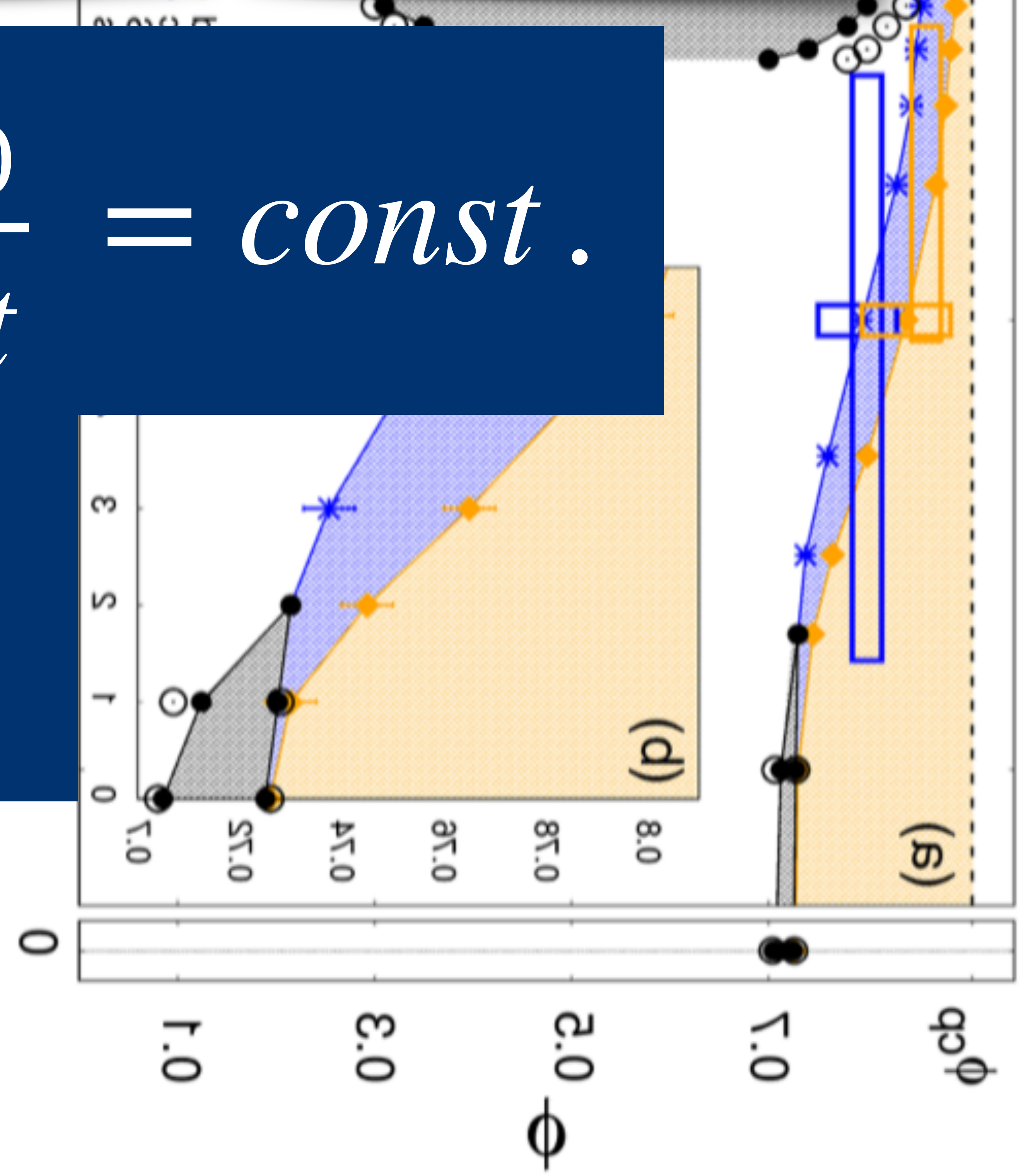
Active Brownian Particles



- J. Klamser, S. Kapfer, W. Krauth, *Nat. Commun.* **9**, Nr. 5045 (2018).
- P. Digregorio, D. Levis, A. Suma, L. F. Cugliandolo, G. Gonnella, I. Pagonabarraga, *PRL* **121**, 098003 (2018).







$$t = n\,dt\,, \qquad v_0 = \frac{\epsilon_0}{dt} = const\,.$$

Carlo

$$dt \to 0$$

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- J. Klamser, S. Kapfer, W. Krauth, *Nat. Commun.* **9**, Nr. 5045 (2018).
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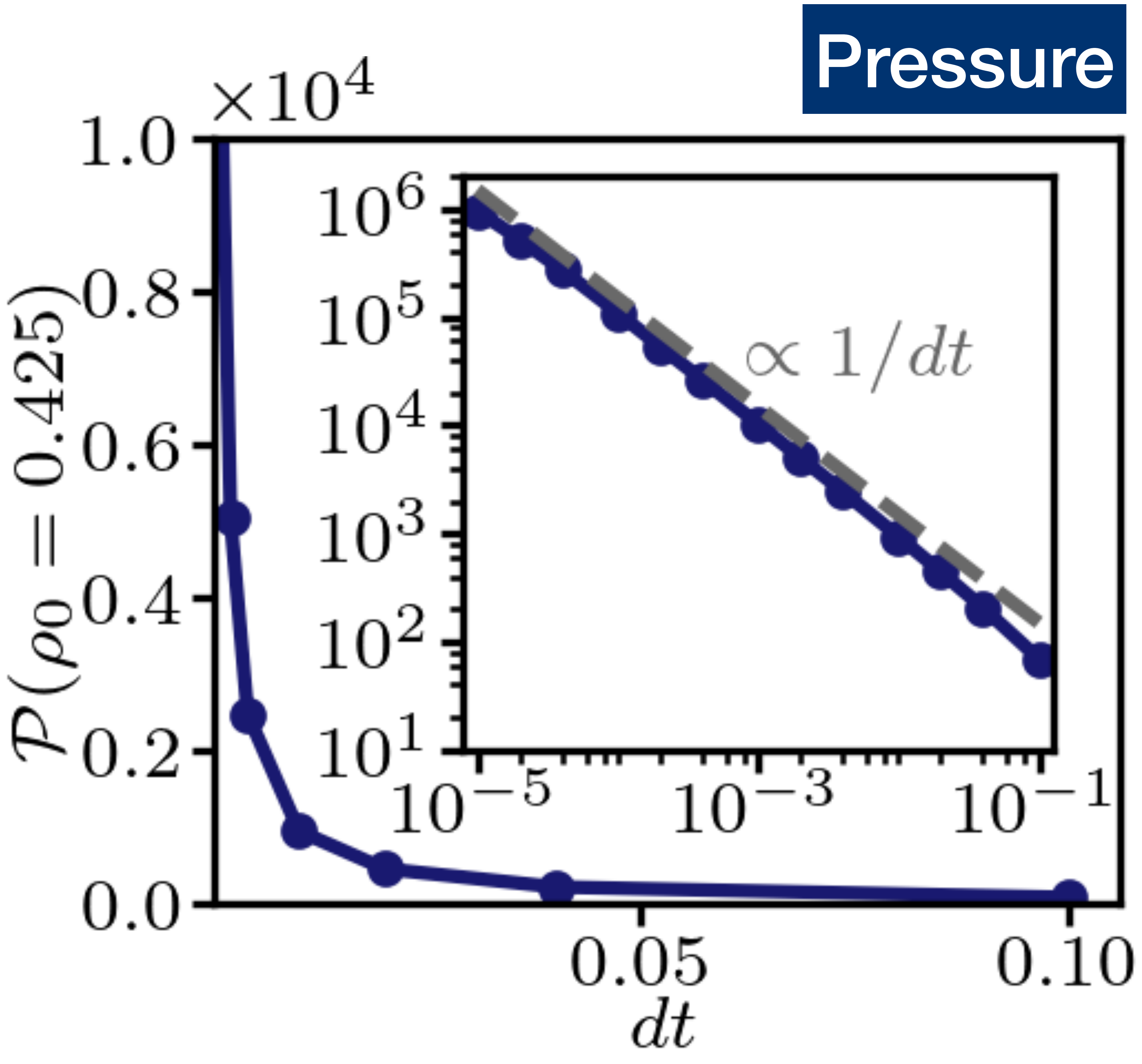
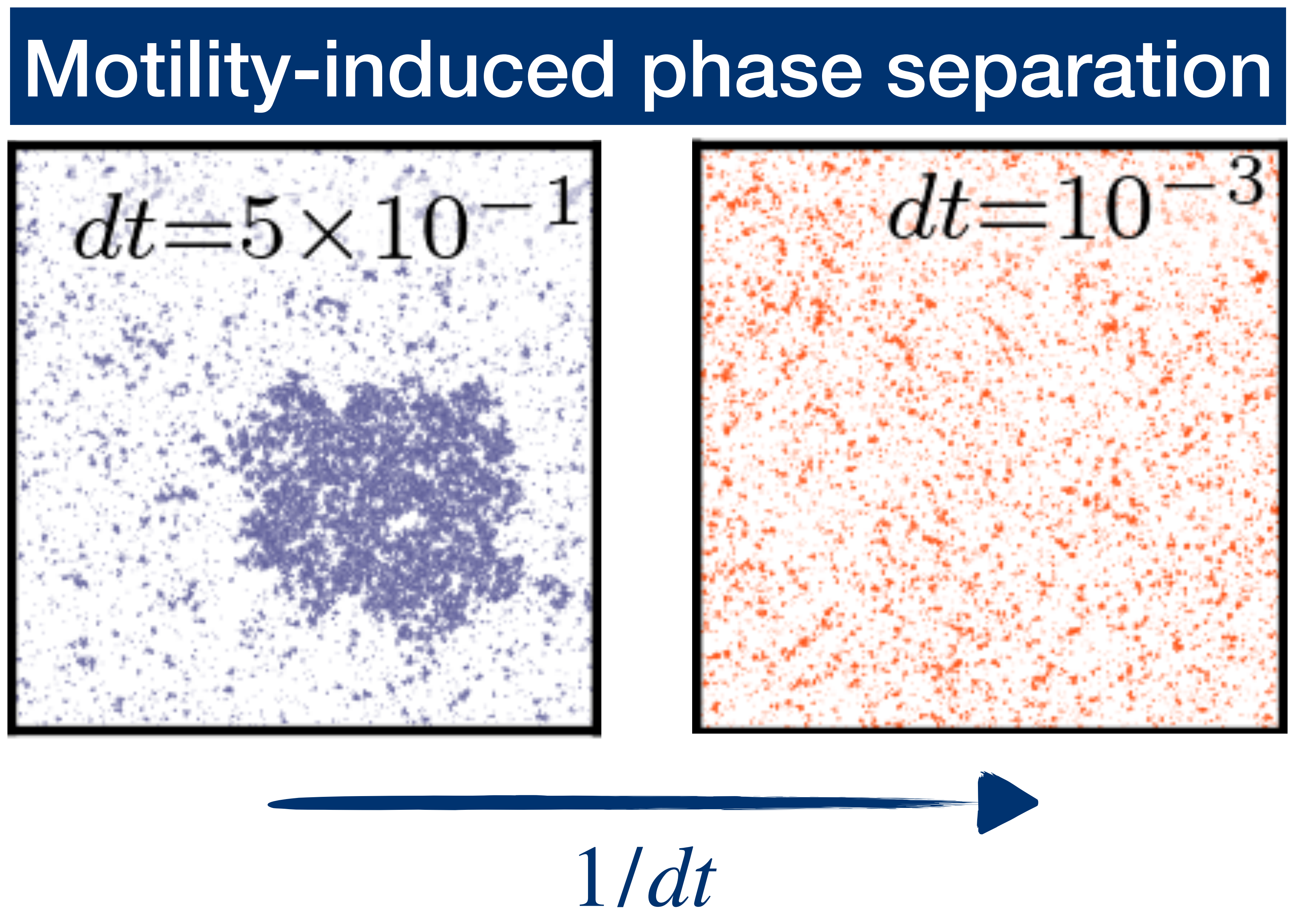
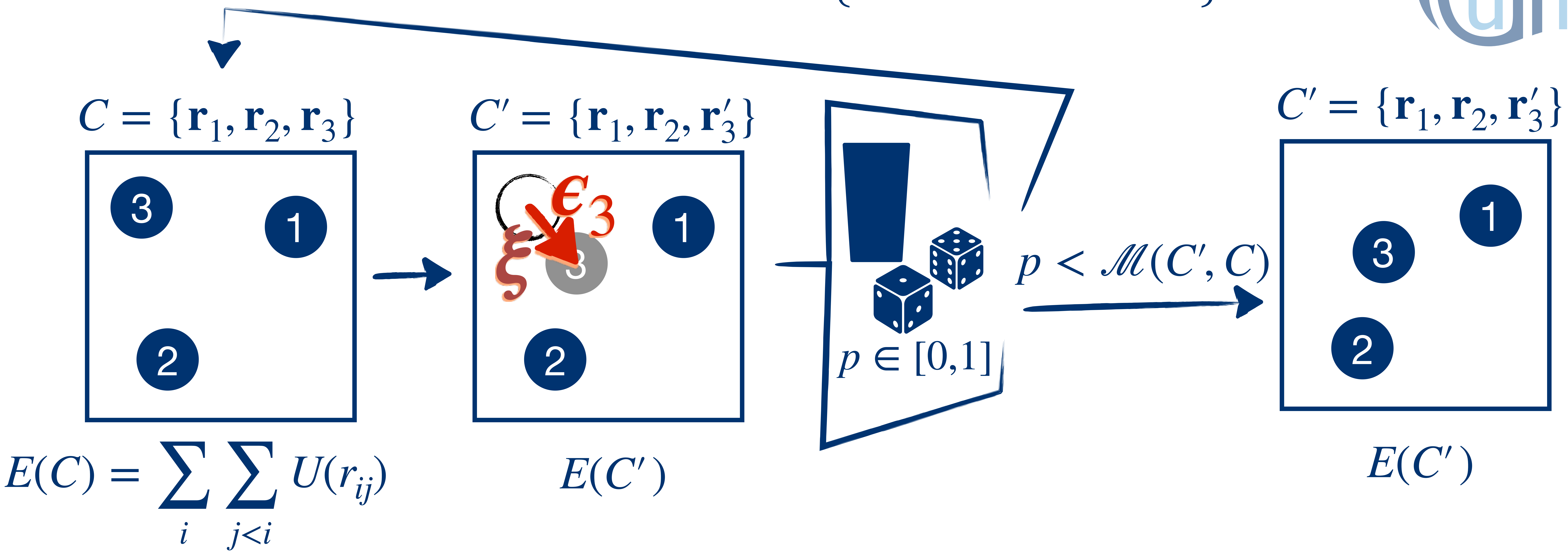


For $dt \to 0$ pressure diverges as $\propto 1/dt$

☹



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



<u>Equilibrium Monte Carlo</u>: $G(\xi)$ = flat measure

<u>Active kinetic MC</u>: $g(\epsilon_i \rightarrow \epsilon'_i)$, time correlated such that $\epsilon'_i \simeq \epsilon_i$

λ - persistence length

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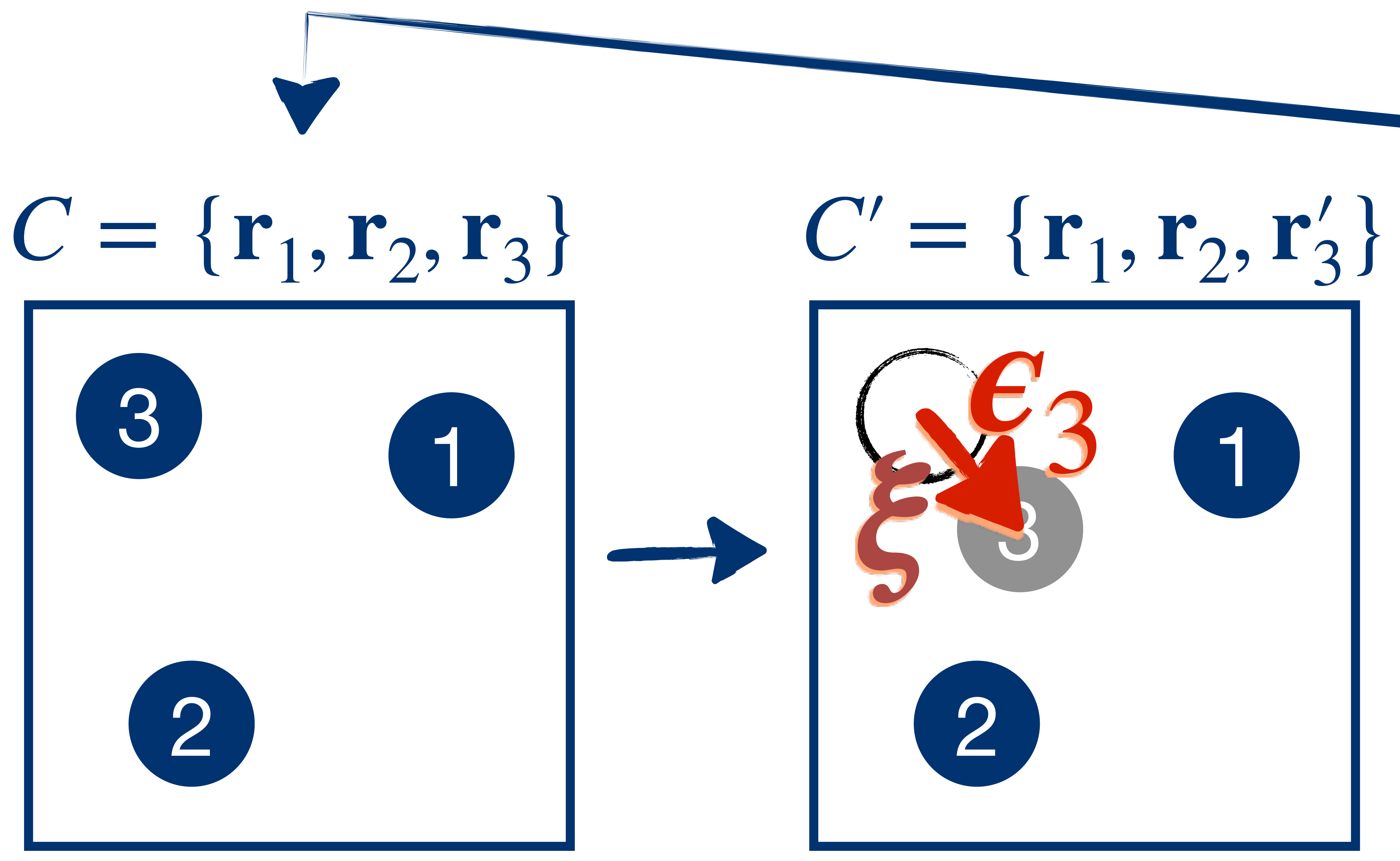
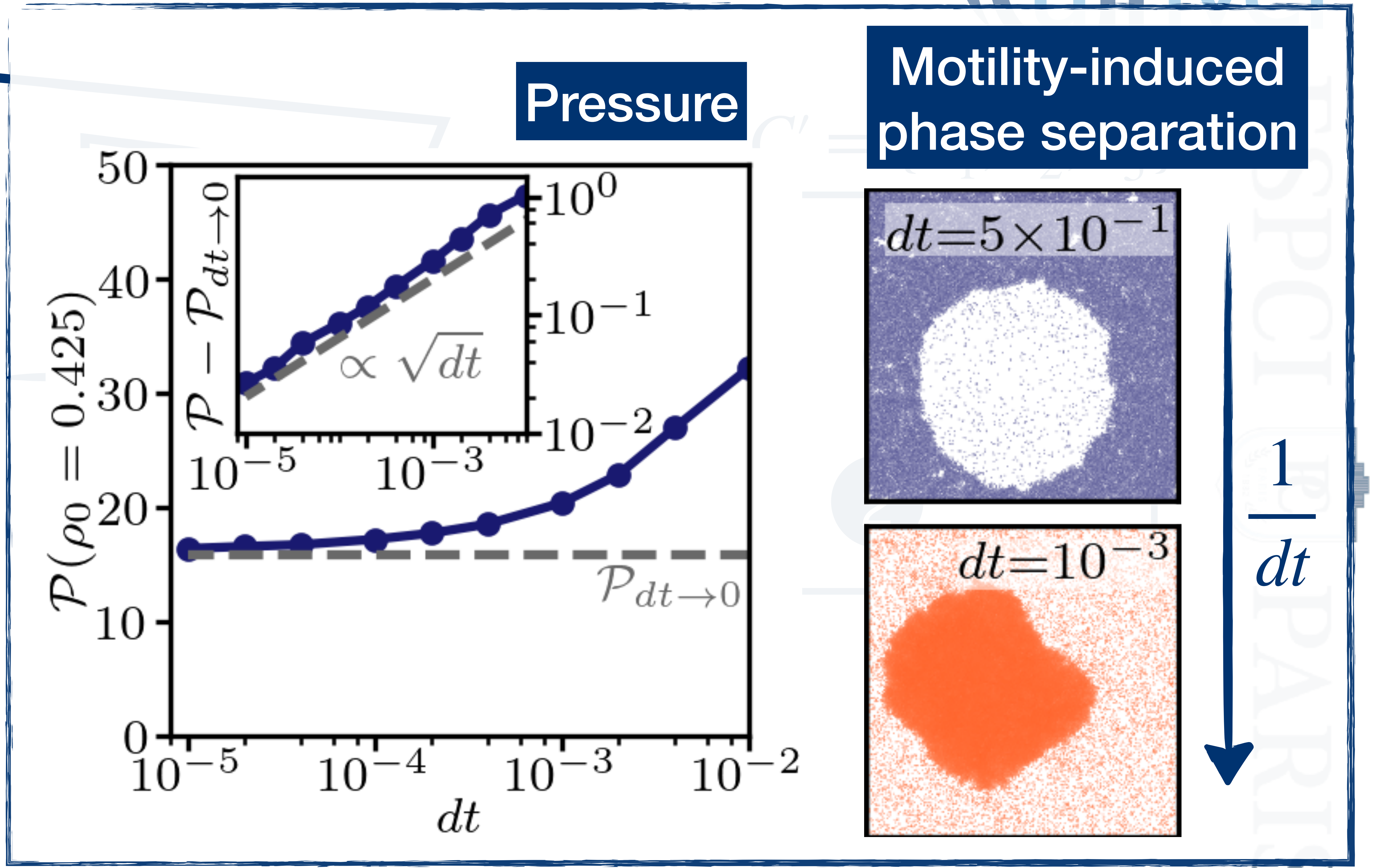


$$E(C) = \sum_i \sum_{j<i} U(r_{ij}) \qquad E(C')$$



<u>Equilibrium Monte Carlo</u>: $G(\xi)$ = flat measure

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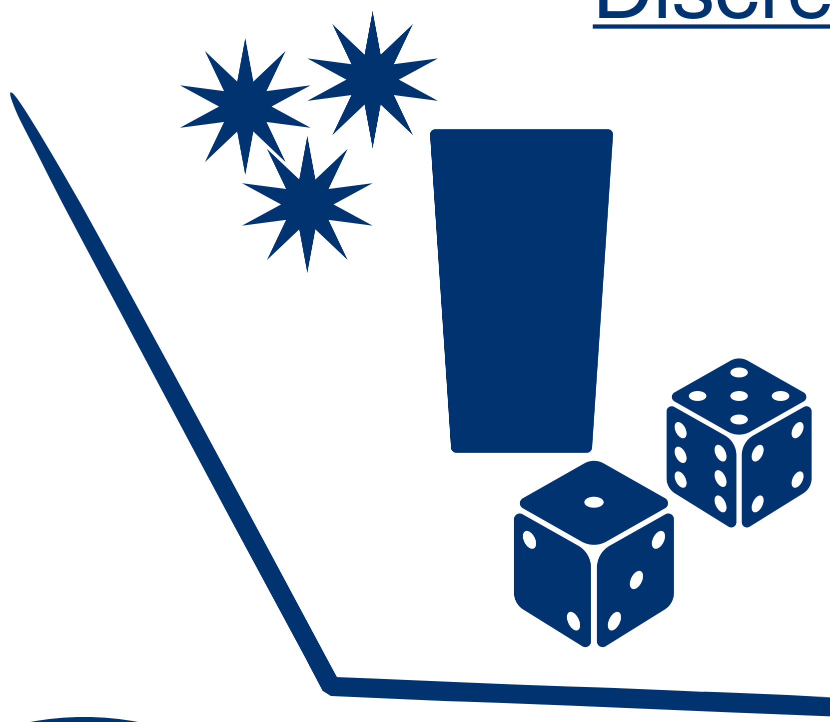


Discrete-time Master equation

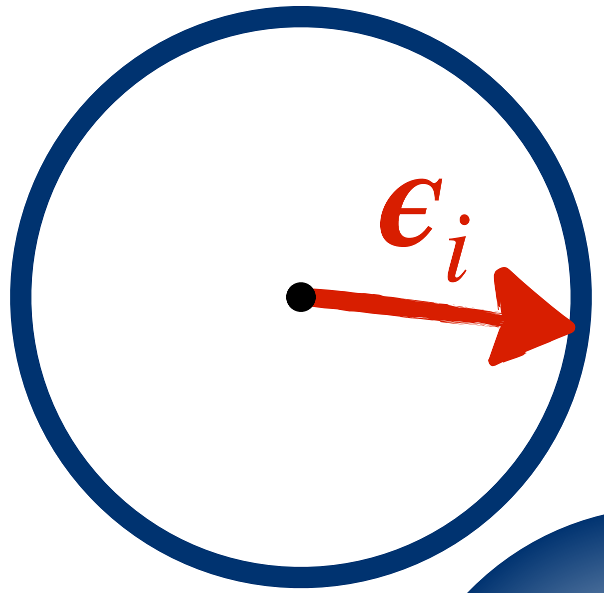
$$P_{n+1}(\mathbf{r}',\epsilon') = \iint M\left(\{\mathbf{r},\epsilon\} \to \{\mathbf{r}',\epsilon'\}\right) P_n(\mathbf{r},\epsilon)\, d\mathbf{r}\, d\epsilon$$

$$M\left(\{\mathbf{r},\epsilon\} \to \{\mathbf{r}',\epsilon'\}\right) = g(\epsilon \to \epsilon')\Big[\alpha\, W\left(\{\mathbf{r},\epsilon/\alpha\} \to \mathbf{r}'\right) + (1-\alpha)\int d\boldsymbol{\xi}\, G(\boldsymbol{\xi})\, W\left(\{\mathbf{r},\boldsymbol{\xi}\} \to \mathbf{r}'\right)\Big]$$

Active Brownian Particles

$$\dot{\boldsymbol{r}}_i = v_0 \boldsymbol{u}(\theta_i) + \sum_{j\neq i} \boldsymbol{F}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right) + \sqrt{2D_t}\boldsymbol{\eta}_i$$

$$\dot{\theta}_i = \sqrt{2D_r}\xi_i$$

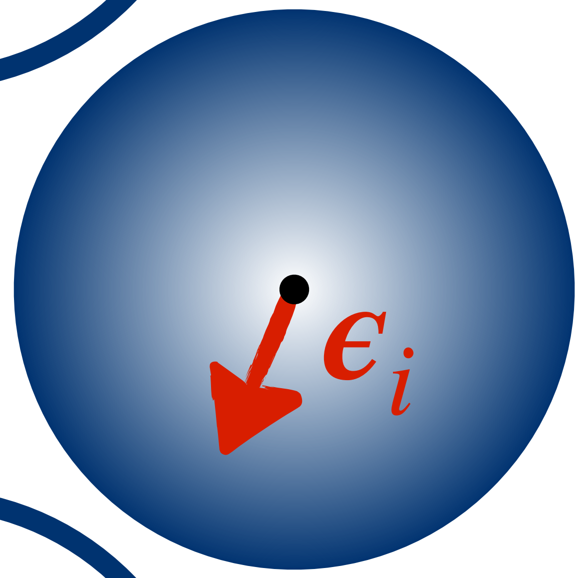


$g(\epsilon_i \to \epsilon_i')$ = random walk on a ring

Active Ornstein-Uhlenbeck Process

$$\dot{\boldsymbol{r}}_i = \boldsymbol{v}_i + \sum_{j\neq i} \boldsymbol{F}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right) + \sqrt{2D_t}\boldsymbol{\eta}_i$$

$$\tau\dot{\boldsymbol{v}}_i = -\boldsymbol{v}_i + \sqrt{2D_v}\xi_i$$

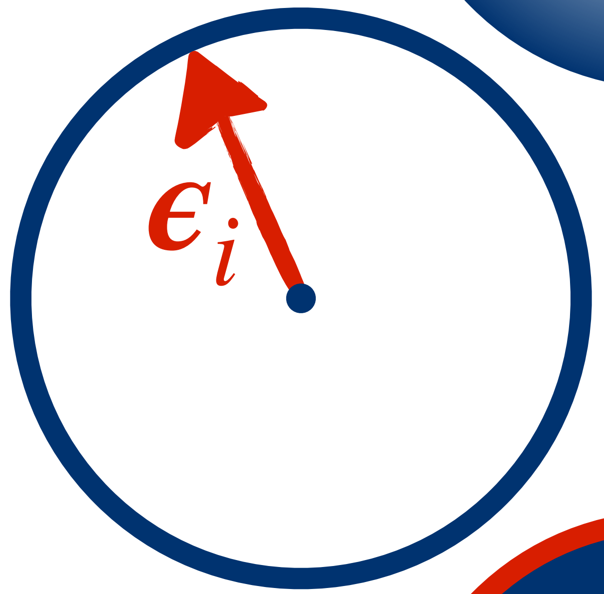


$g(\epsilon_i \to \epsilon_i')$ = random walk in a harmonic potential

Run-And-Tumble Particles

$$\dot{\boldsymbol{r}}_i = v_0 \boldsymbol{u}(\theta_i) + \sum_{j\neq i} \boldsymbol{F}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right) + \sqrt{2D_t}\boldsymbol{\eta}_i$$

$\theta_i(t) = \theta_i(t-\Delta t)$, with $P(\Delta t)$

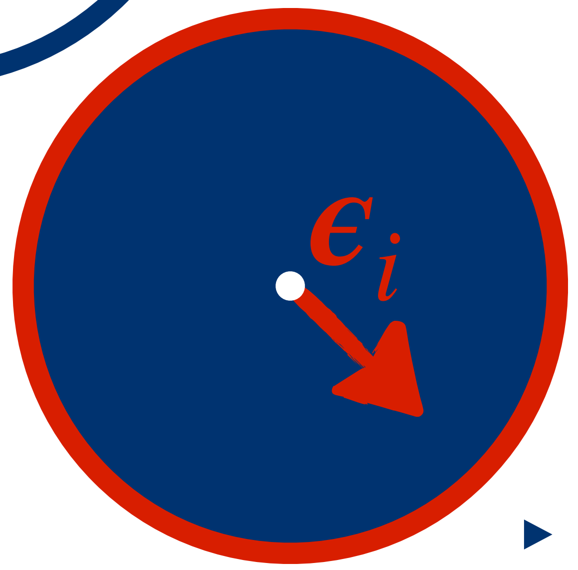


$g(\epsilon_i \to \epsilon_i')$ = instantaneous jumps on a circle under some finite rate

Active Random-Acceleration Process

$$\dot{\boldsymbol{r}}_i = \boldsymbol{v}_i + \sum_{j\neq i} \boldsymbol{F}\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right) + \sqrt{2D_t}\boldsymbol{\eta}_i$$

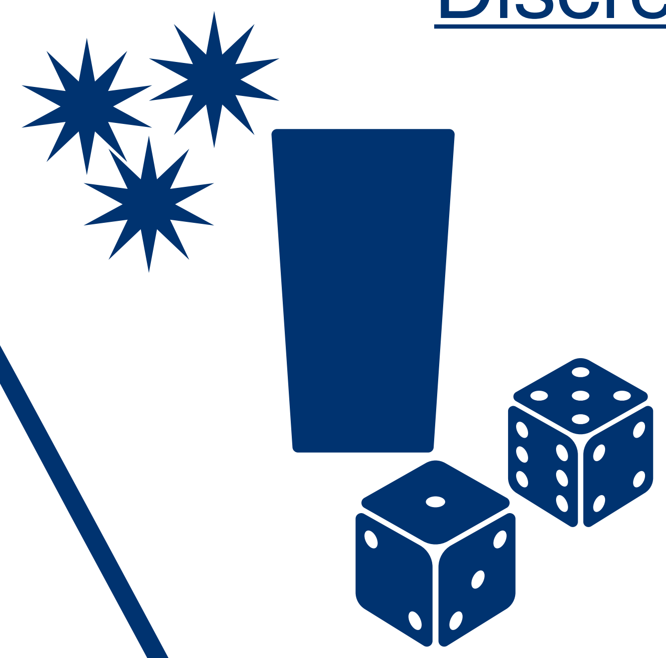
$\dot{\boldsymbol{v}}_i = \sqrt{2D_v}\xi_i$ reflecting boundaries at v_0



$g(\epsilon_i \to \epsilon_i')$ = random walk inside a circle with reflecting boundaries

- J. U. Klamser, O. Dauchot, J. Tailleur, PRL 127, 150602 (2021).

Discrete-time Master equation



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Active Brownian Particles

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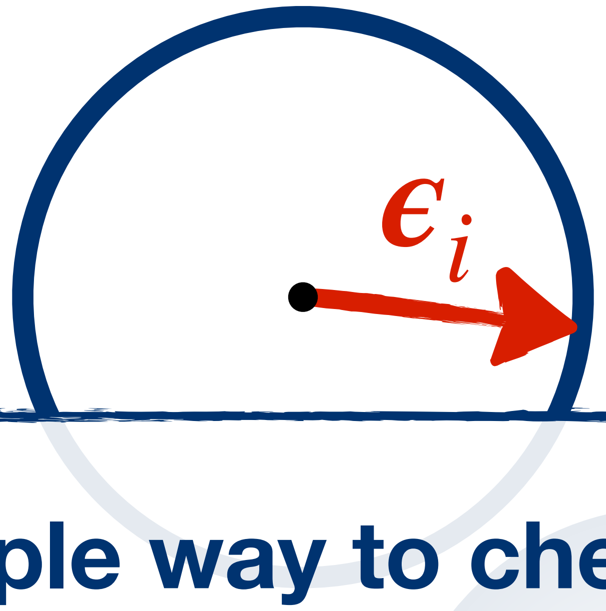
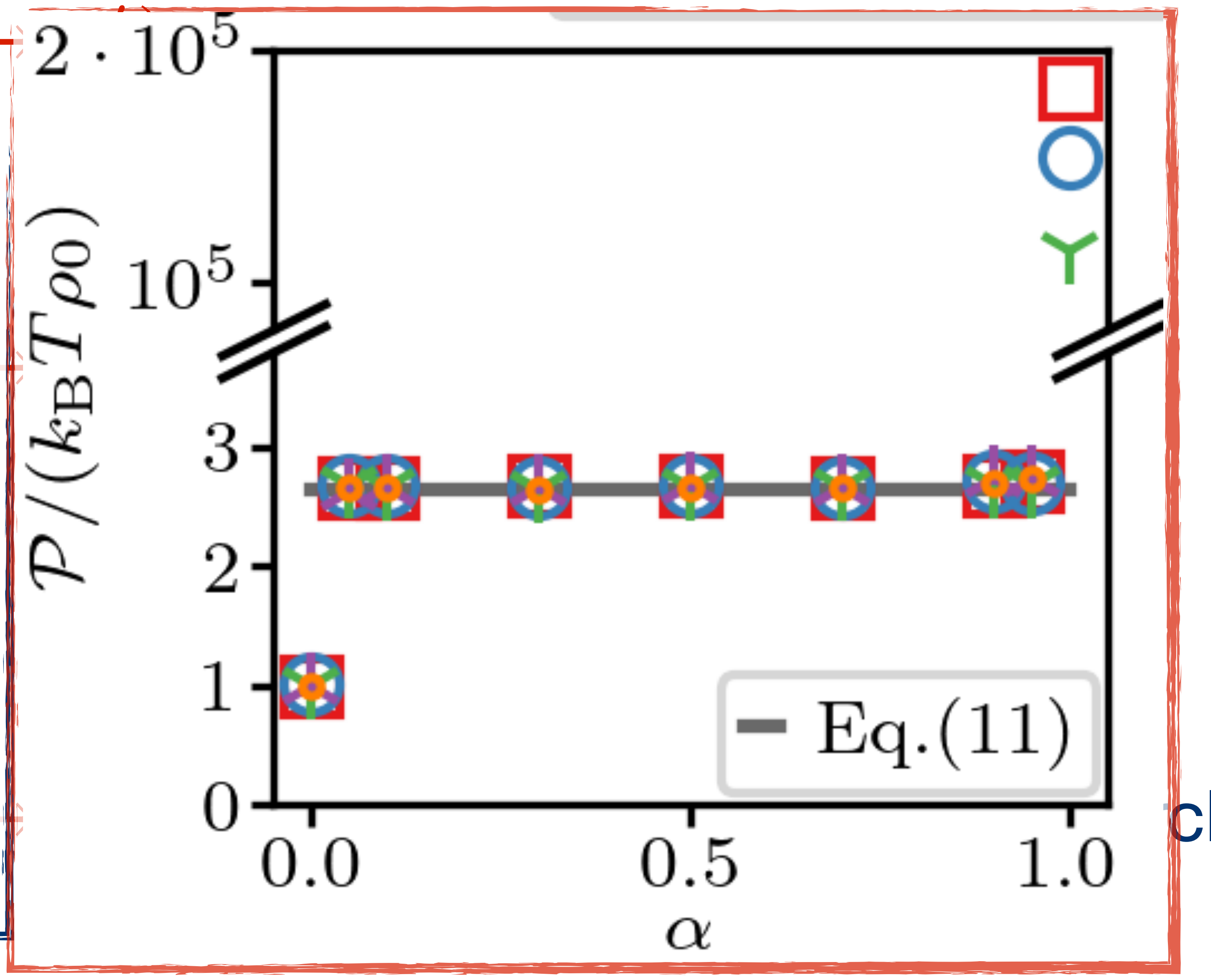


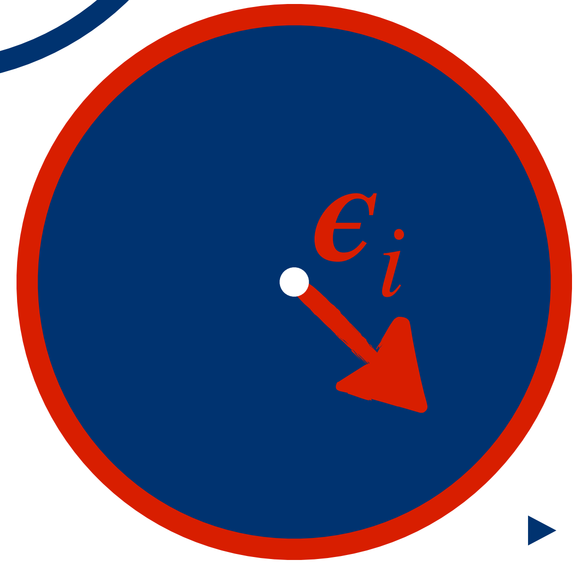
Simple way to check?

$$\mathscr{P}_{\text{ideal}} = \mathscr{P}_{\text{passive}} + \mathscr{P}_{\text{active}}$$

$\mathscr{P}_{\text{passive}} \to \rho_{\text{bulk}} k_B T$, $\mathscr{P}_{\text{active}} \to \propto \rho_{\text{bulk}}$

- Solon, A., Fily, Y., Baskaran, A. et al., *Nature Phys* **11**, 673–678 (2015).





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