EAJSSP 2025

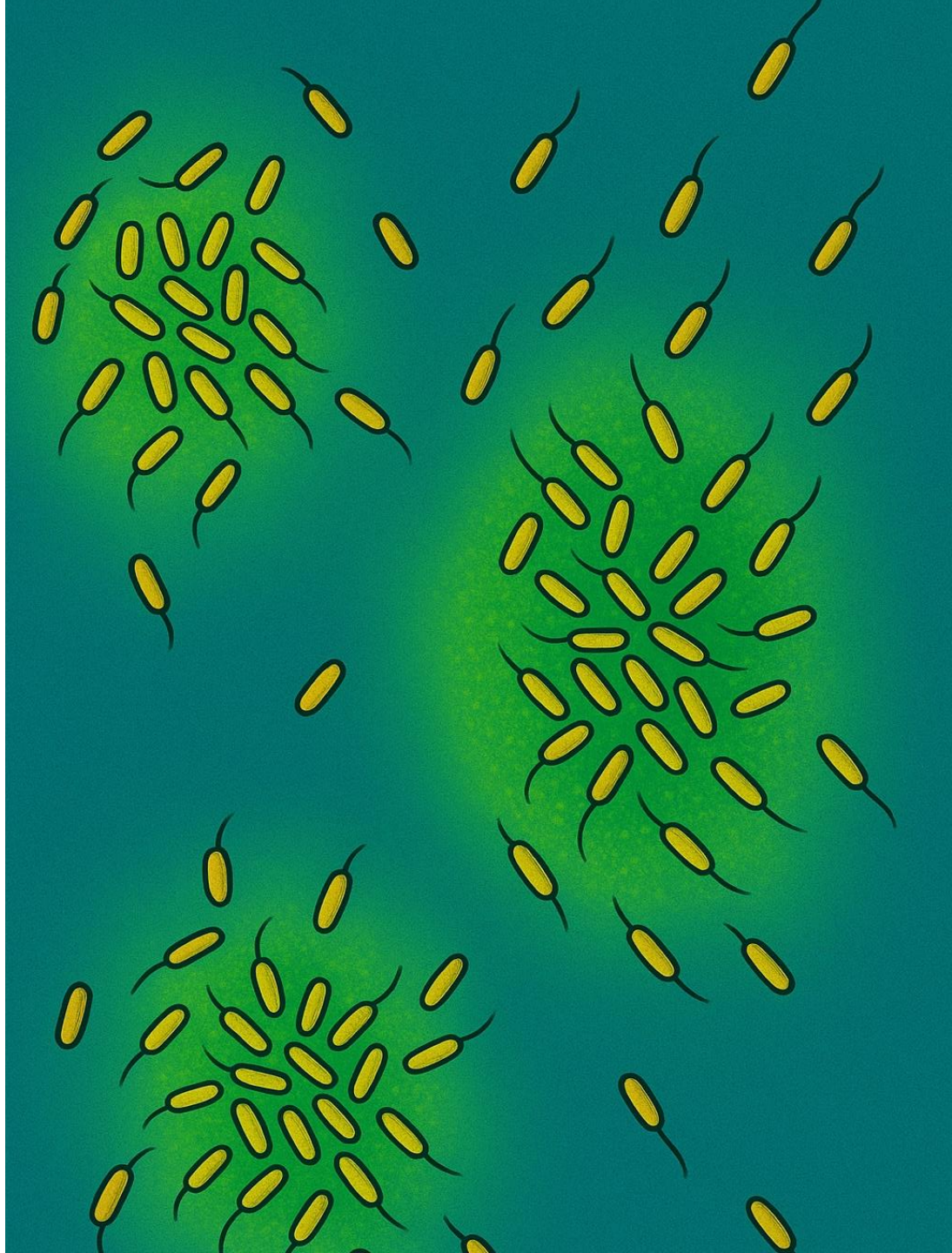
Pattern formation of fuel-consuming and chemokinetic active particles

Commun. Phys. **8**, 288 (2025)

Euijoon Kwon, Yongjae Oh, and **Yongjoo Baek**

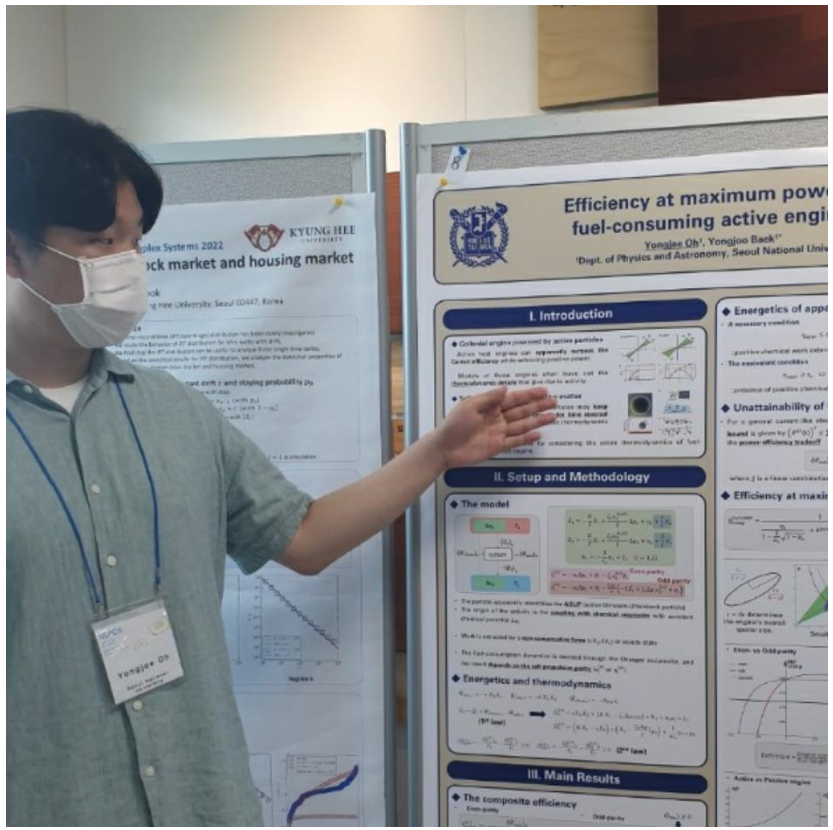
Department of Physics and Astronomy

Seoul National University



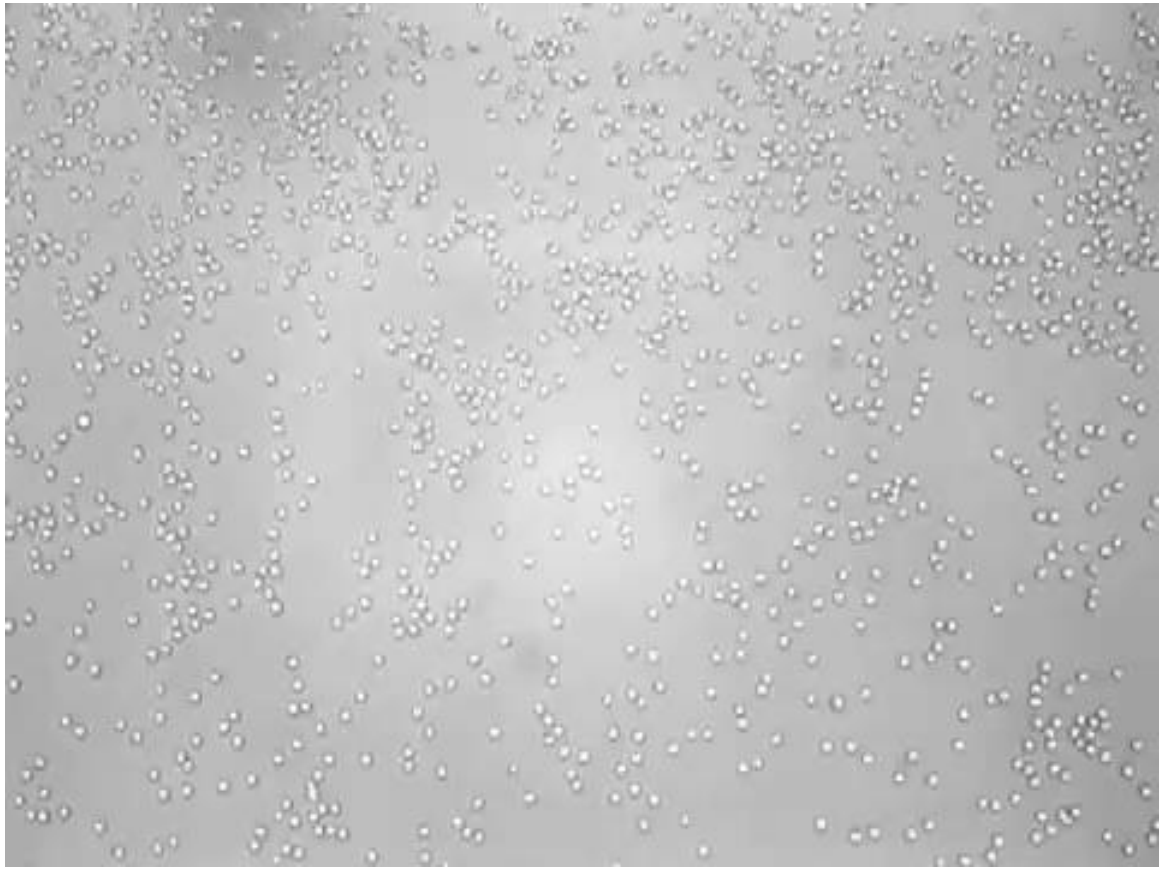


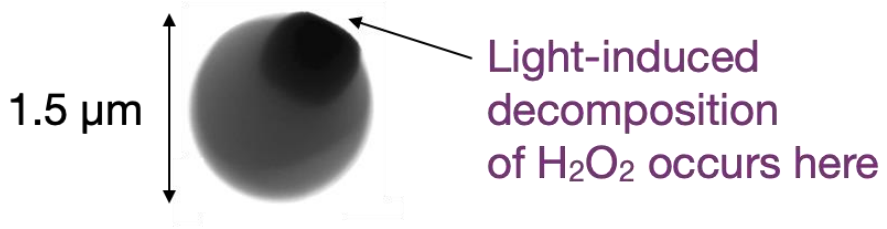
Euijoon Kwon

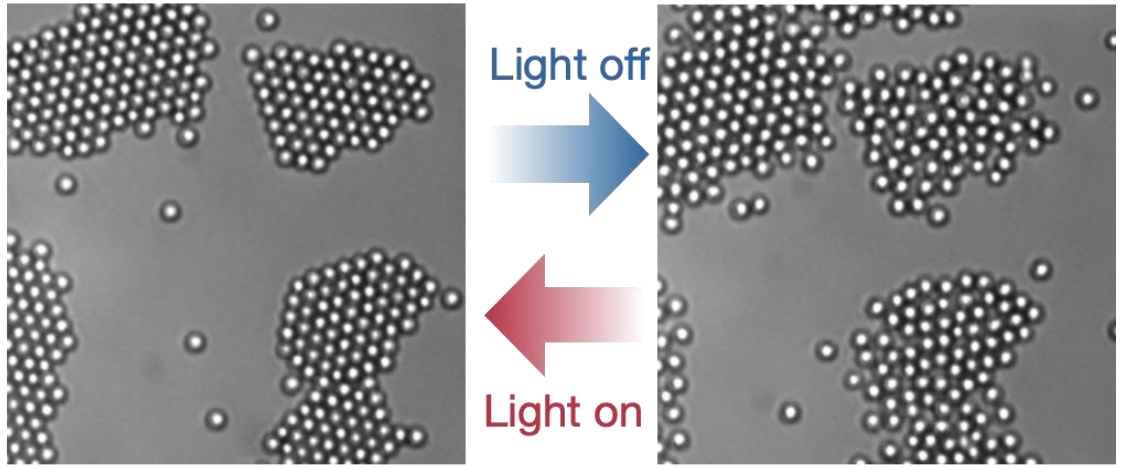


Yongjae Oh

Motility-induced phase separation (MIPS)

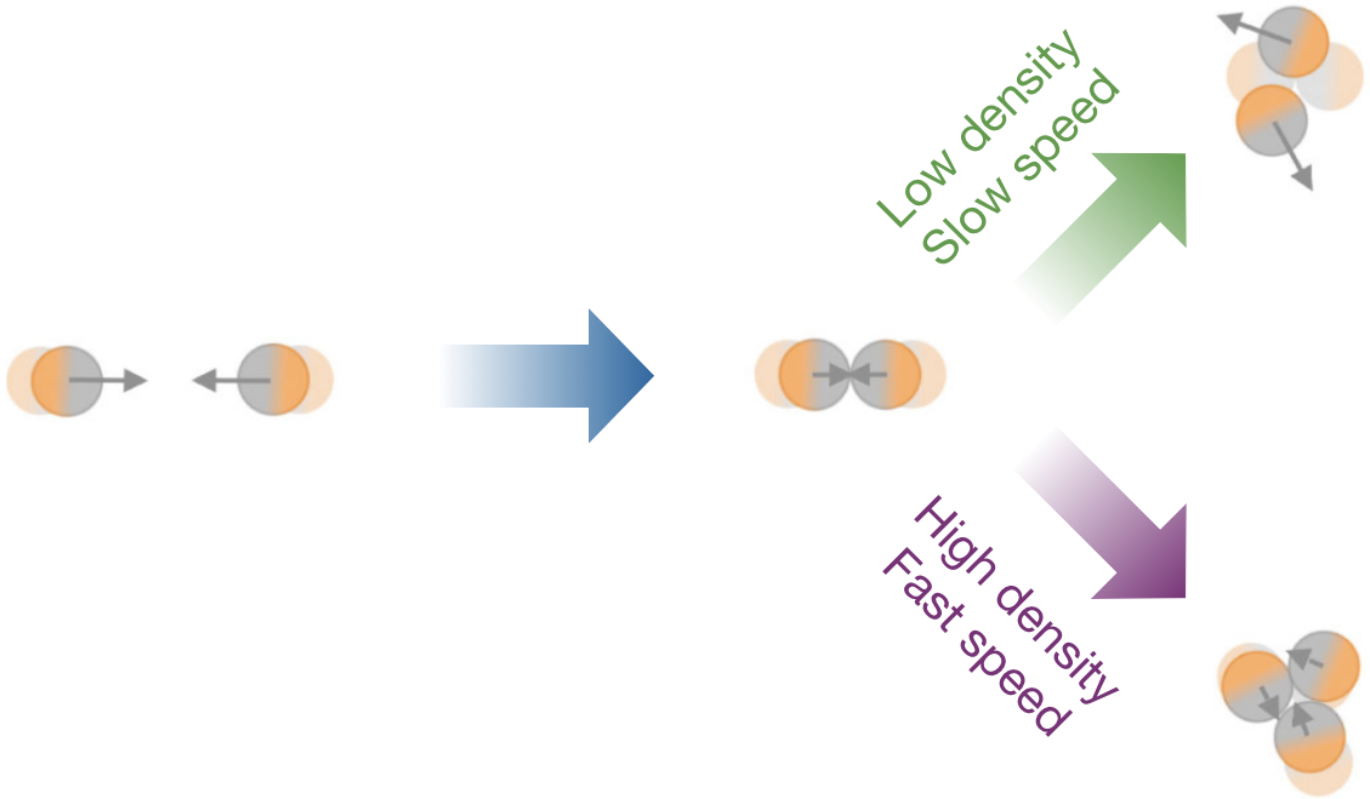






- Even without interparticle attraction, active particles with short-range repulsion can phase separate due to their motility.

Kinetic picture of MIPS



Single phase



Phase separation

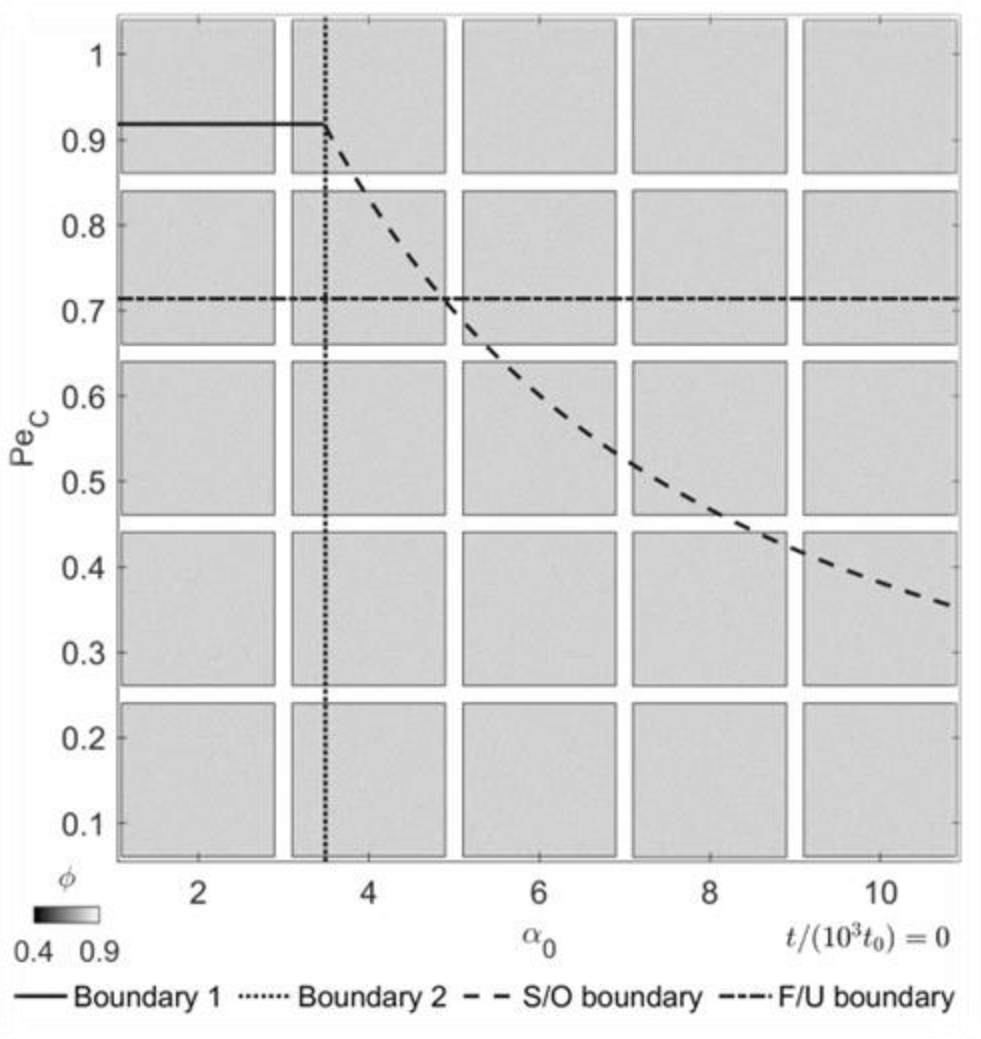
- Positive feedback between increased density & reduced speed leads to phase separation.

Traditional models of MIPS assume that the **self-propulsion force** evolves according to some independent random process with the magnitude staying constant:

$$\dot{\boldsymbol{r}}_k = \mu\, v\, \hat{\mathbf{e}}_k + \sqrt{2\mu T}\, \xi_k$$

But what if self-propulsion is coupled to chemicals produced/consumed by the particles?

MIPS with chemotaxis



$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \boldsymbol{J},$$

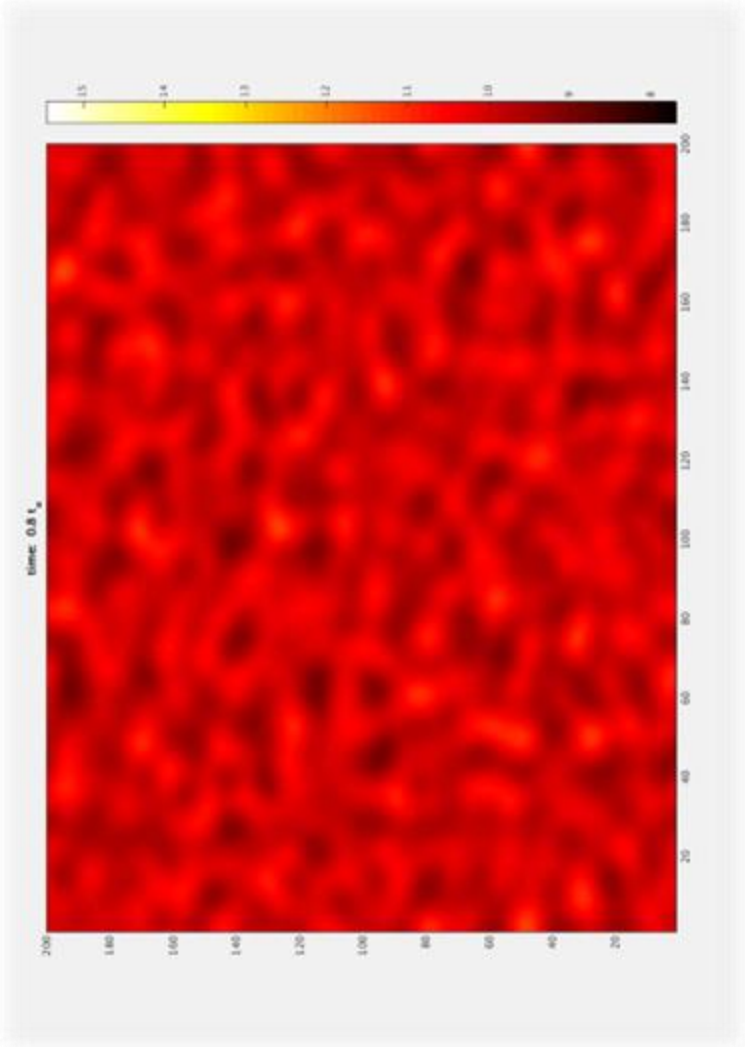
$$\boldsymbol{J} = \underbrace{-M_0 \phi \nabla \left(\tilde{\mu}_h(\phi, \mathrm{Pe}_R) - \kappa \nabla^2 \phi \right)}_{\text{MIPS}} + \underbrace{\chi_0 \phi \nabla f(\tilde{c})}_{\text{chemotaxis}},$$

$$\frac{\partial \tilde{c}}{\partial t} = D_c \nabla^2 \tilde{c} - k \phi g(\tilde{c}) + S,$$

- Chemoattraction with chemical consumption suppresses MIPS, arrests phase separation, and creates traveling waves.

Zhao, Košmrlj, & Datta, *Phys. Rev. Lett.* (2023)

MIPS with chemotaxis



$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \boldsymbol{J},$$

$$\boldsymbol{J} = \underbrace{-M_0 \phi \nabla \left(\tilde{\mu}_h(\phi, \mathrm{Pe}_R) - \kappa \nabla^2 \phi \right)}_{\text{MIPS}} + \underbrace{\chi_0 \phi \nabla f(\tilde{c})}_{\text{chemotaxis}},$$

$$\frac{\partial \tilde{c}}{\partial t} = D_c \nabla^2 \tilde{c} - k \phi g(\tilde{c}) + S,$$

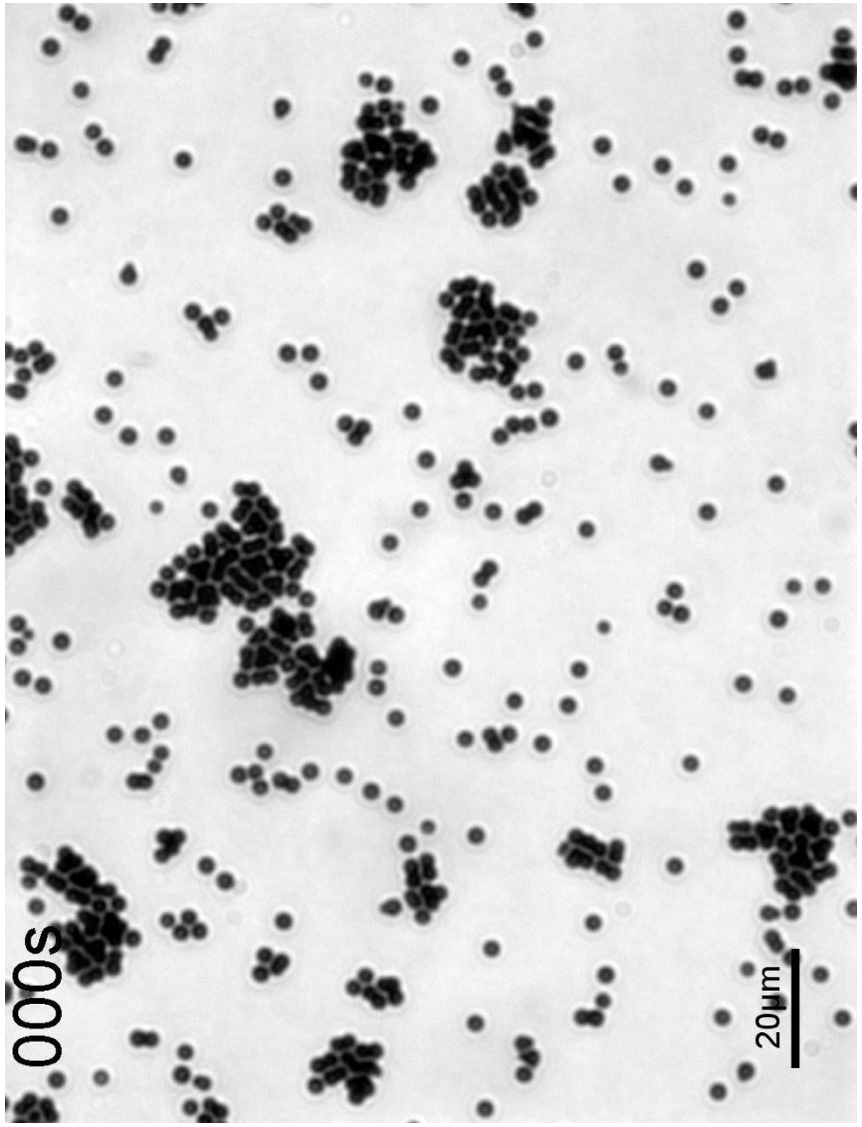
- Chemoattraction with chemical consumption suppresses MIPS, arrests phase separation, and creates traveling waves.

  Zhao, Košmrlj, & Datta, *Phys. Rev. Lett.* (2023)

- Chemorepulsion with chemical production generates microphase separation, blinking clusters, and traveling waves.

  Liebchen *et al.*, *Phys. Rev. Lett.* (2015)

MIPS with chemotaxis



- If two halves of a diffusiophoretic Janus particle have different mobility coefficients, such particles also exhibit chemotaxis.

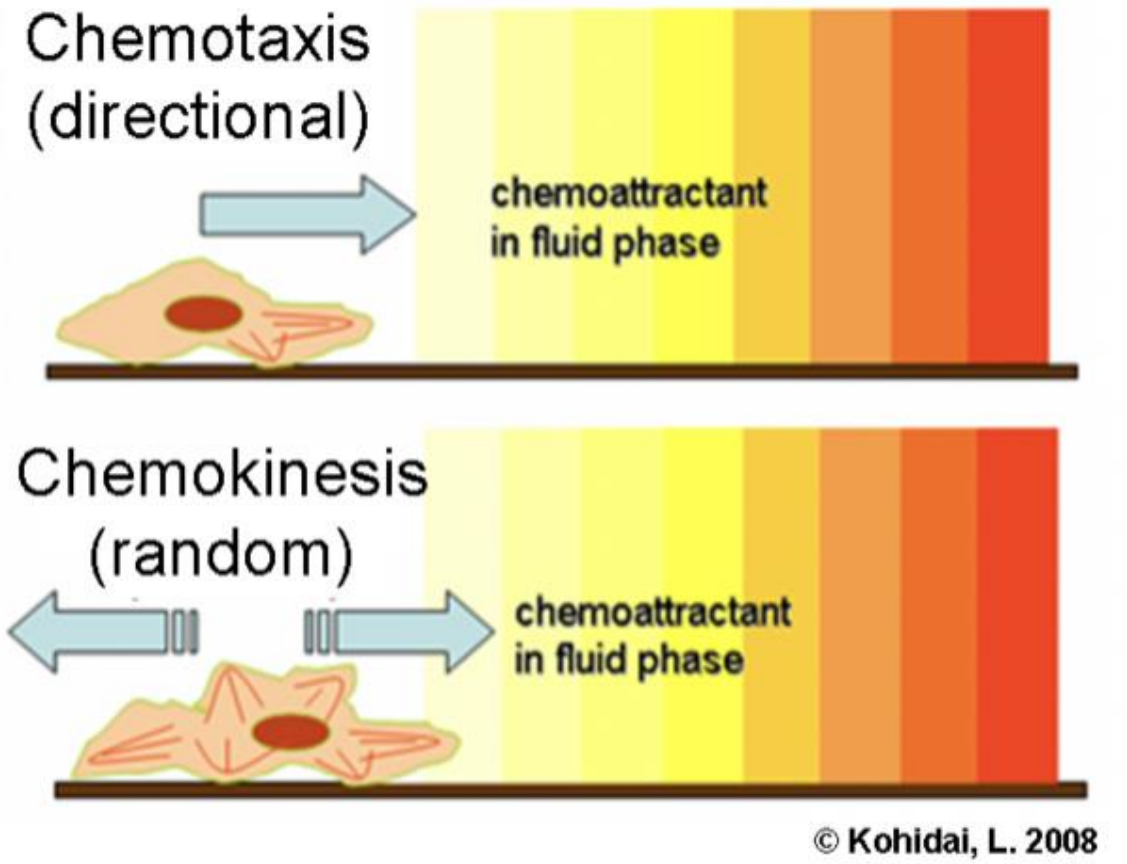
  Anderson, *Annu. Rev. Fluid Mech.* (1989)

- For spherical Pt-Au Janus particles fueled by H_2O_2, effective chemorepulsion with fuel consumption arrests phase separation and generates dynamic clustering.

  Experiment: Theurkauff *et al.*, *Phys. Rev. Lett.* (2012)

  Theory: Pohl & Stark, *Phys. Rev. Lett.* (2014)

Chemotaxis vs. chemokinesis



- **Chemotaxis**: direction of self-propulsion aligns or anti-aligns with the chemical concentration gradient

- **Chemokinesis:** motility of particles change depending on the chemical concentration

Chemokinesis without chemotaxis

- There are cells which exhibit strong chemokinesis but very weak chemotaxis: neutrophils in the aged people, human endothelial cells after CMG2 gene is blocked, etc.

  Sapey *et al*., *Blood* (2014)

  Cryan *et al*., *Angiogenesis* (2022)

- Diffusiophoretic Pt-polystyrene Janus particles, electrophoretic Pt-Au rods exhibit chemokinetic response to their fuel (H_2O_2) but very little chemotaxis.

  Howse *et al*., *Phys. Rev. Lett.* (2007)

  Moran *et al*., *Sci. Rep.* (2021)

- For diffusiophoretic Janus particles, chemotaxis is negligible if the mobility coefficients of the two halves of each particle are not very different.

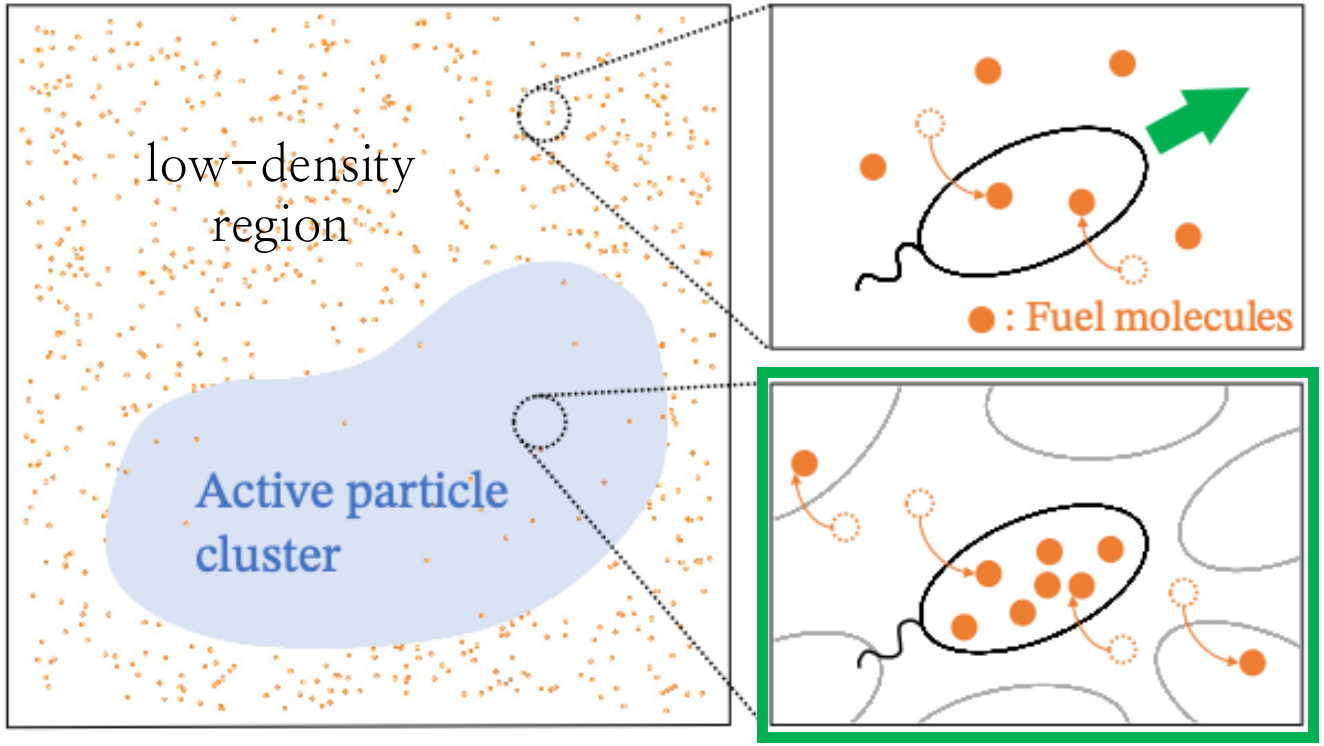
  Anderson, *Annu. Rev. Fluid Mech.* (1989)

Q. How is MIPS altered when active particles are chemokinetic but not chemotactic to their fuel?

Two regimes of chemical consumption

- **BMR (Basal metabolic regime)**

  : chemical consumption is proportional to **density of the active particles**.



Inside the **particle cluster**

: depletion of chemicals

→ weaker self-propulsion

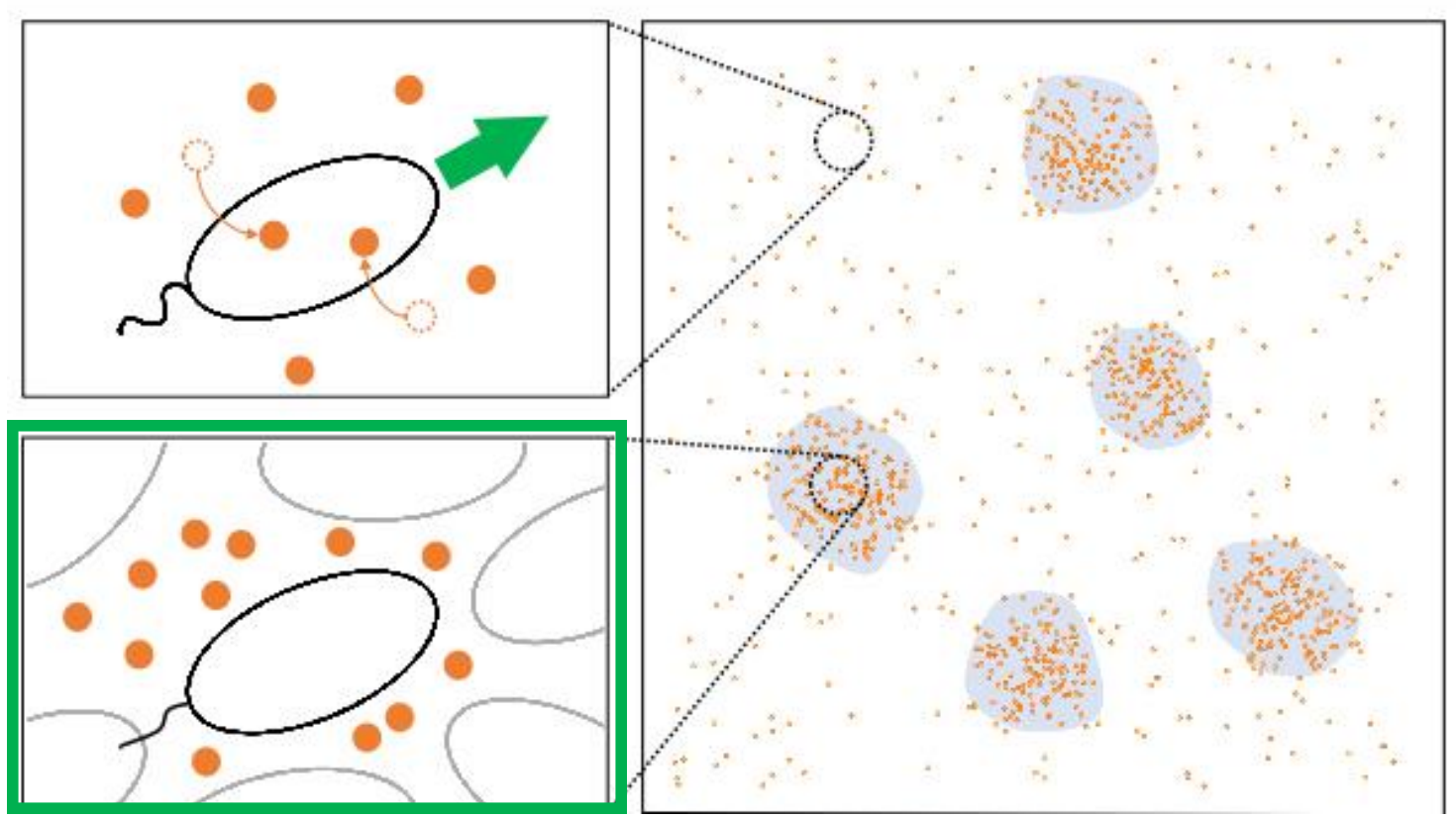
→ difficult to escape the cluster

∴ **MIPS is enhanced**

Two regimes of chemical consumption

- **AMR (Active metabolic regime)**

  : chemical consumption is proportional to the **actual distances** traveled by particles.



Inside the **particle cluster**

: little actual motion of particles

→ unused chemicals

→ stronger self-propulsion

→ easier evaporation

∴ **Phase separation is suppressed**

Our model: particle-based version

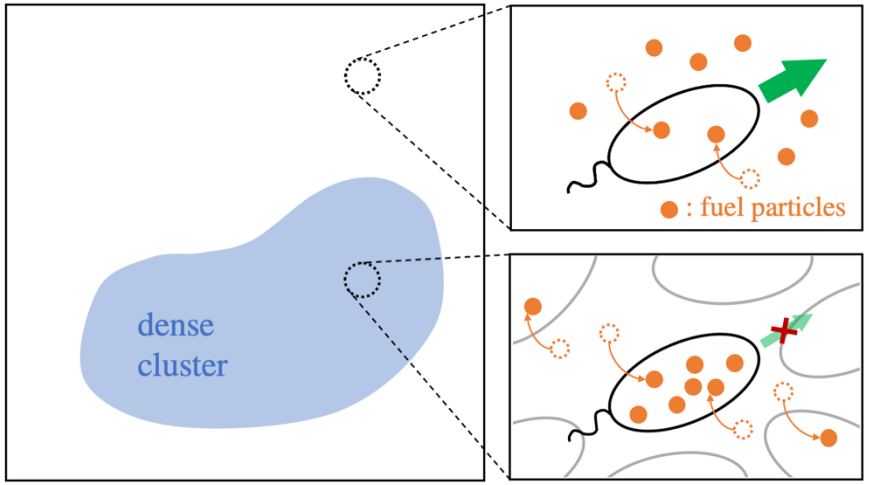
particle: $$\dot{\boldsymbol{r}}_k = \mu\, v\big(n(\boldsymbol{r}_k,t)\big)\,\hat{\mathbf{e}}_k - \sum_{k'\neq k} \mu\nabla_k V(|\boldsymbol{r}_k - \boldsymbol{r}_{k'}|) + \sqrt{2\mu T}\,\xi_k,$$

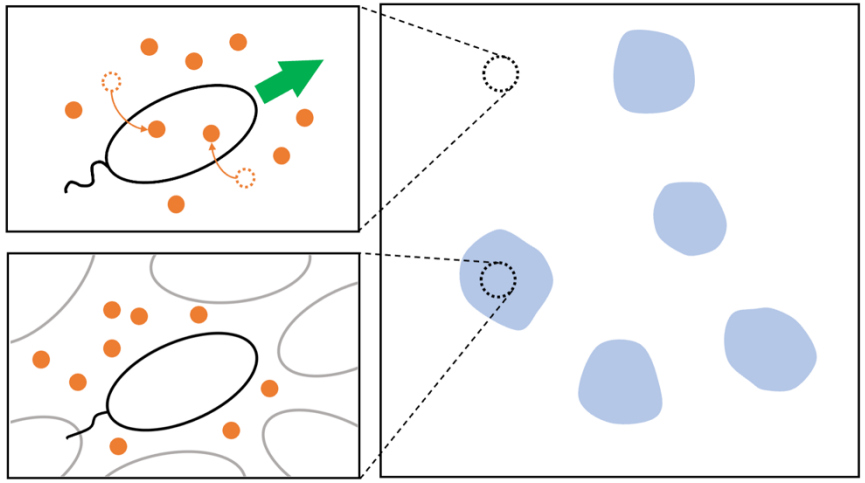
Concentration-dependent self-propulsion

Angular diffusion

Short-range repulsion

chemical: $$\dot{n}(\boldsymbol{r},t) = D_c\,\nabla^2 n + I - \lambda\, f(n,\{\boldsymbol{r}_k\})$$ **chemical consumption**





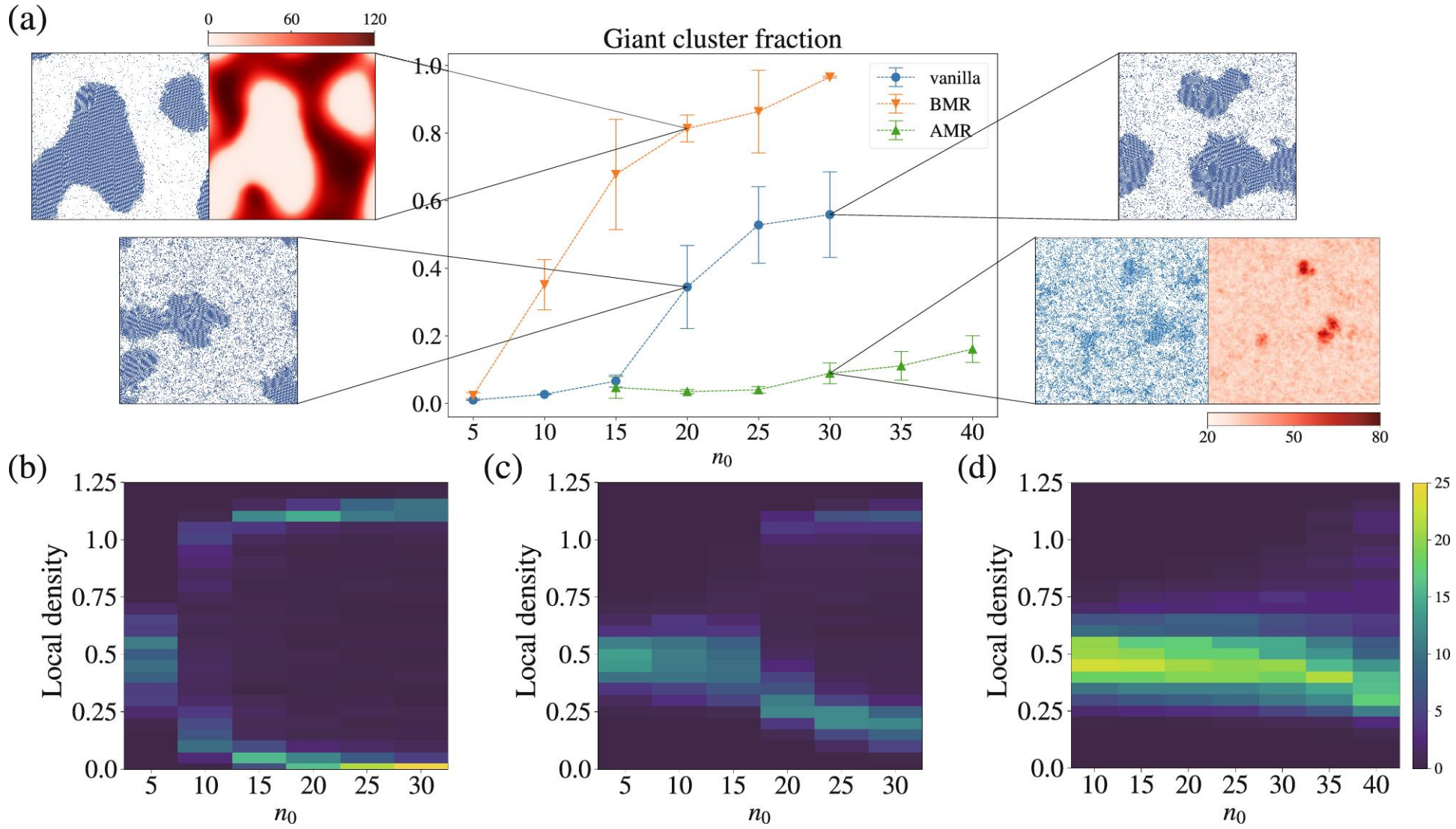
$$f(n,\{\boldsymbol{r}_k\}) = \int d^2\boldsymbol{r}' n(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}') \sum_{k'=1}^{N} \delta(\boldsymbol{r}' - \boldsymbol{r}_{k'})$$

BMR

$$f(n,\{\boldsymbol{r}_k\}) = \int d^2\boldsymbol{r}' n(\boldsymbol{r})\,\delta(\boldsymbol{r}-\boldsymbol{r}') \sum_{k'=1}^{N} \dot{\boldsymbol{r}}_{k'}\cdot\hat{\mathbf{e}}_{k'}\,\delta(\boldsymbol{r}' - \boldsymbol{r}_{k'})$$

AMR

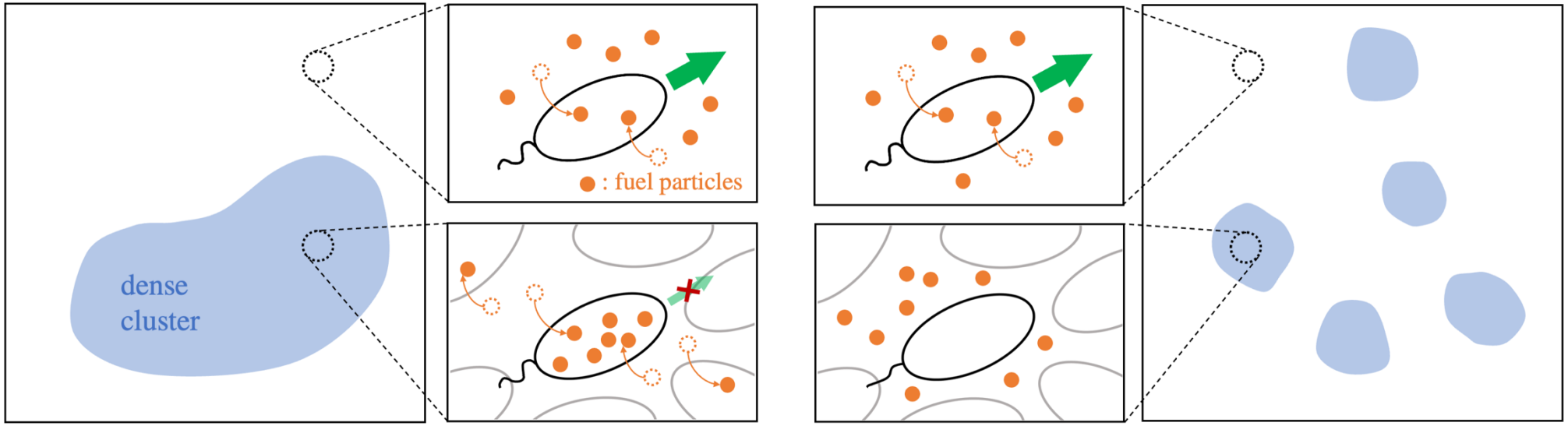
Particle-based models (short-range repulsion)



- The intuition is basically correct, but can we understand this theoretically?

Our model: hydrodynamic version

[Derived via the coarse-graining scheme of Bialké, Löwen, and Speck, *Europhys. Lett.* (2013)]



Basal Metabolic Regime (BMR) Active Metabolic Regime (AMR)

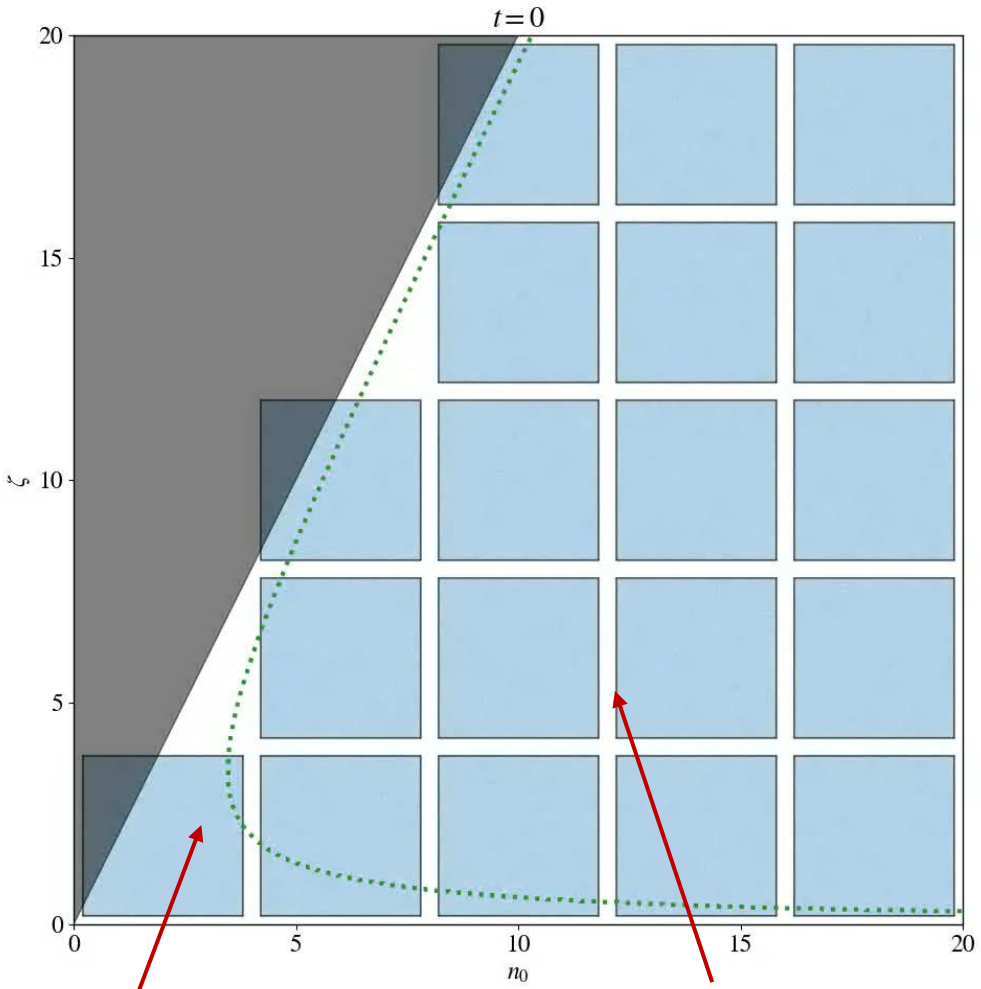
$$\dot{\rho}(\boldsymbol{r},t) = \boldsymbol{\nabla}\cdot\left[D\,\boldsymbol{\nabla}\rho + \frac{v(\rho,n)}{2D_{\mathrm{r}}}\boldsymbol{\nabla}[v(\rho,n)\rho] - \kappa\boldsymbol{\nabla}(\boldsymbol{\nabla}^2\rho)\right], \qquad v(\rho,n) = \alpha n - \zeta\rho$$

effective self-propulsion

deceleration due to repulsion

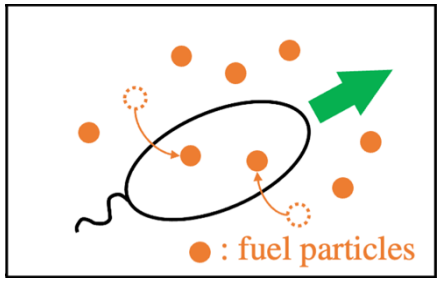
$$\dot{n}(\boldsymbol{r},t) = D_c\boldsymbol{\nabla}^2 n + I - \begin{cases} \lambda\,\rho\,n & \text{(BMR)} \\ \lambda\,\rho\,v(\rho,n)\,n & \text{(AMR)} \end{cases}$$

BMR phase diagram

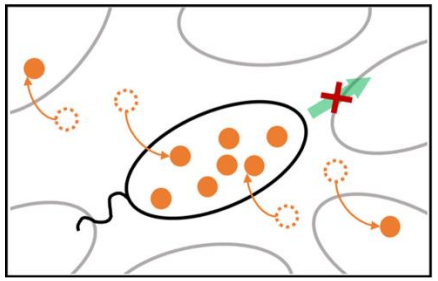


homogeneous phase

stationary MIPS (time-oscillatory)



low-density region



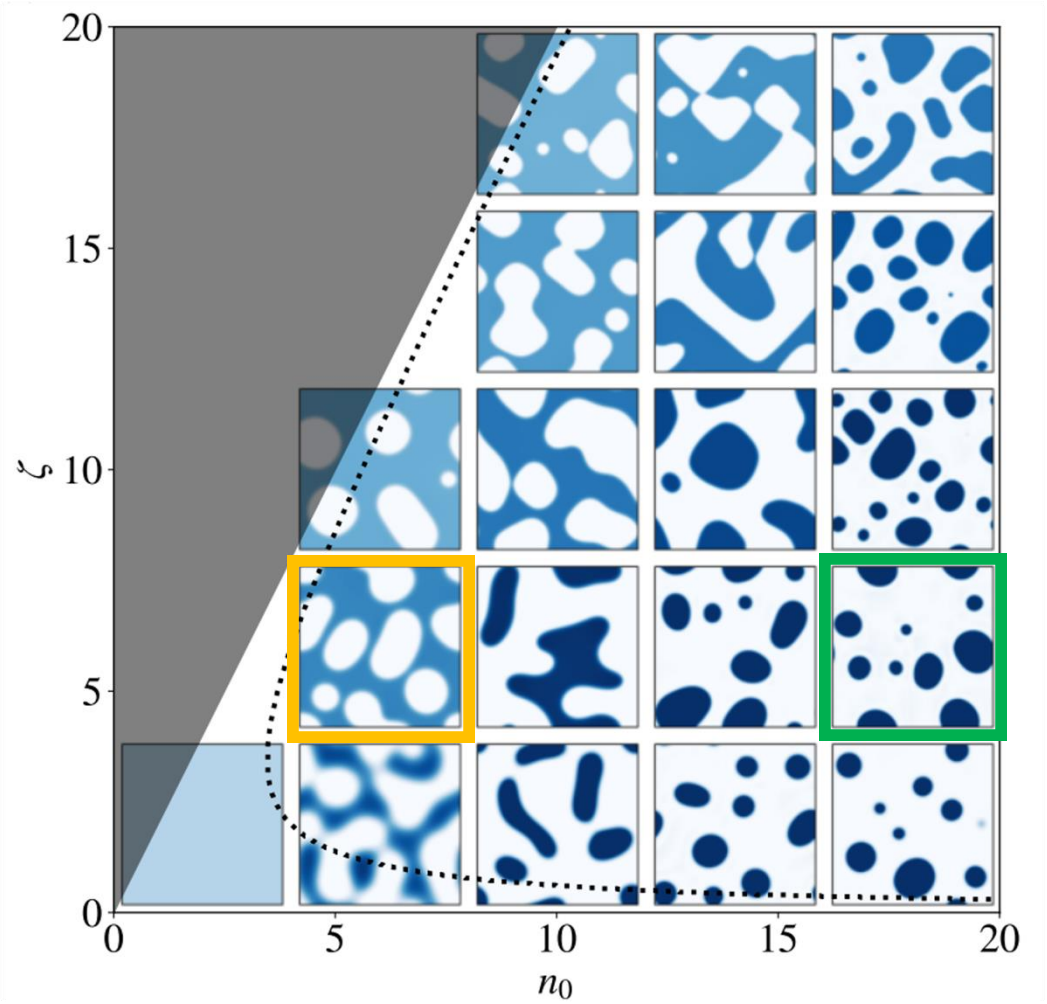
dense cluster
: wastes fuel → difficult to escape

- n_0: global chemical concentration
- ζ: deceleration rate

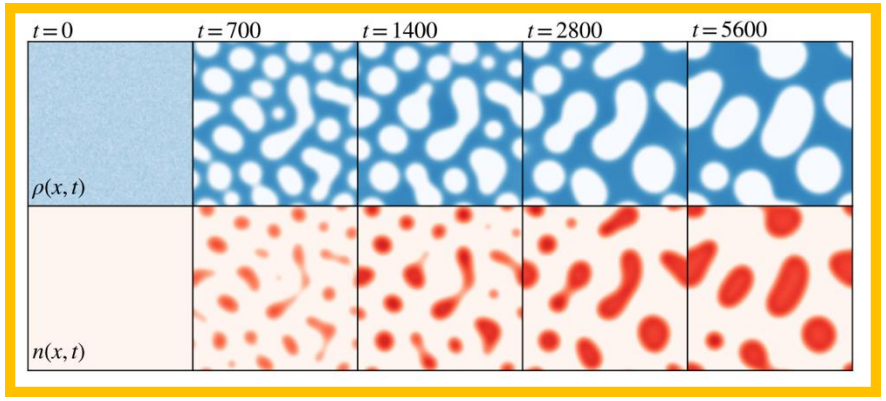
$$(v_{\text{eff}} = \alpha n_0 - \rho_0 \zeta)$$

- Phase boundary correctly predicted by the linear stability analysis
- BMR facilitates the MIPS.

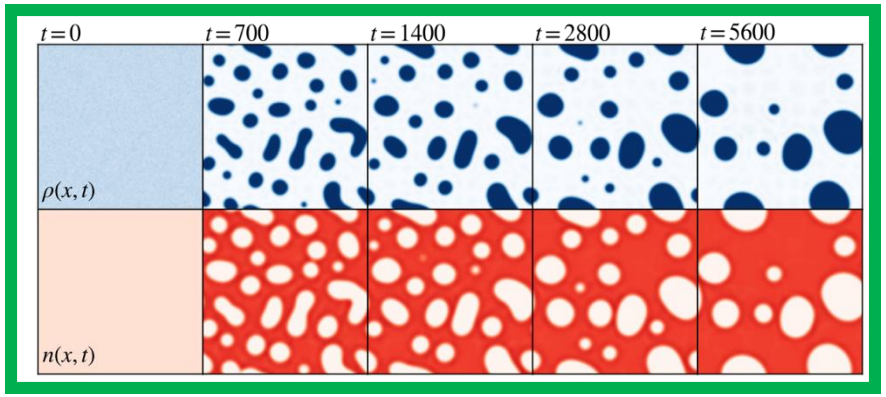
BMR phase separates



Time-lapse images



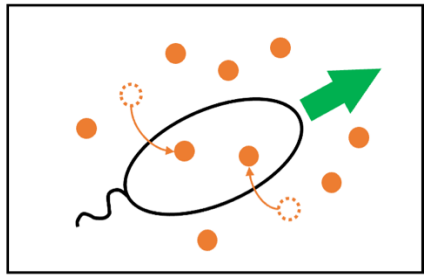
- **Bubbles** are initially formed, and then merges into larger bubbles, leading to a global phase separation.



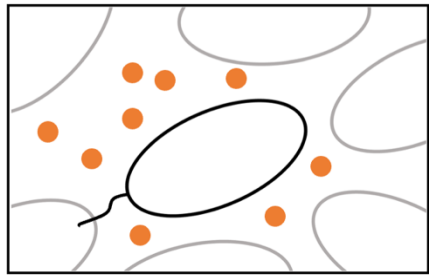
- **Clusters** are initially formed, and then merges into larger clusters, leading to a global phase separation.

AMR phase diagram

- **AMR** (active metabolic regime)

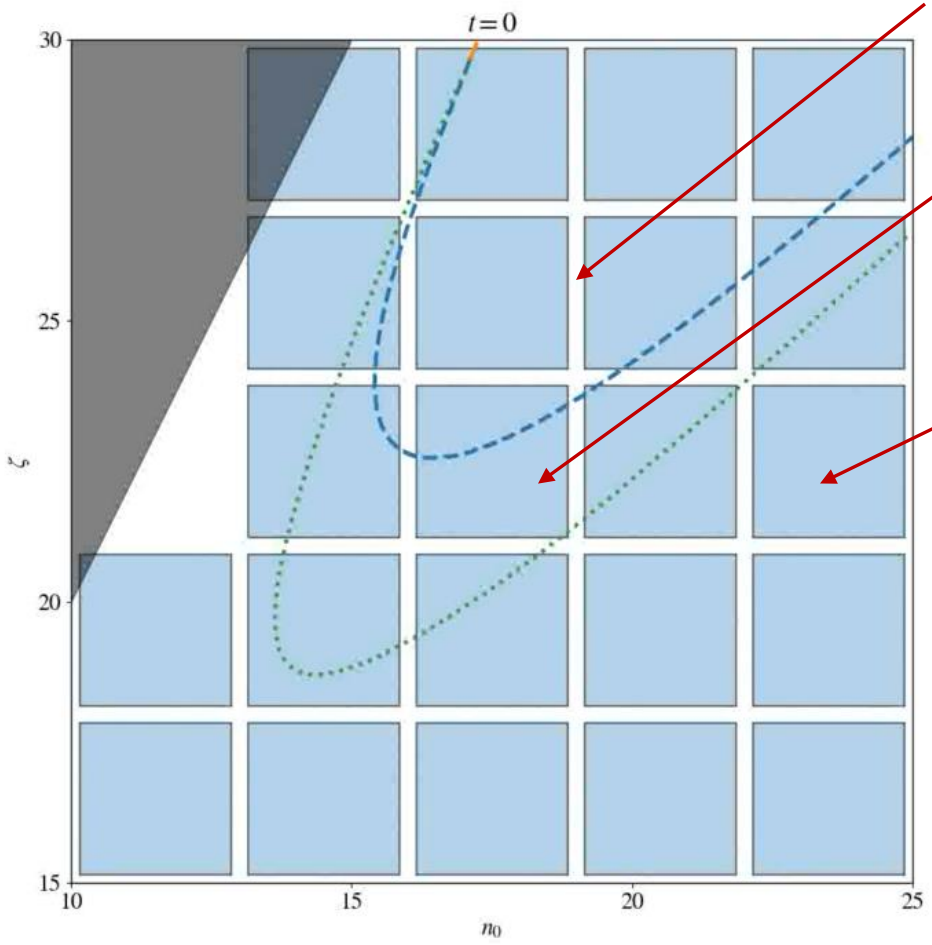


low-density region



dense cluster

: saves fuel → likely to escape

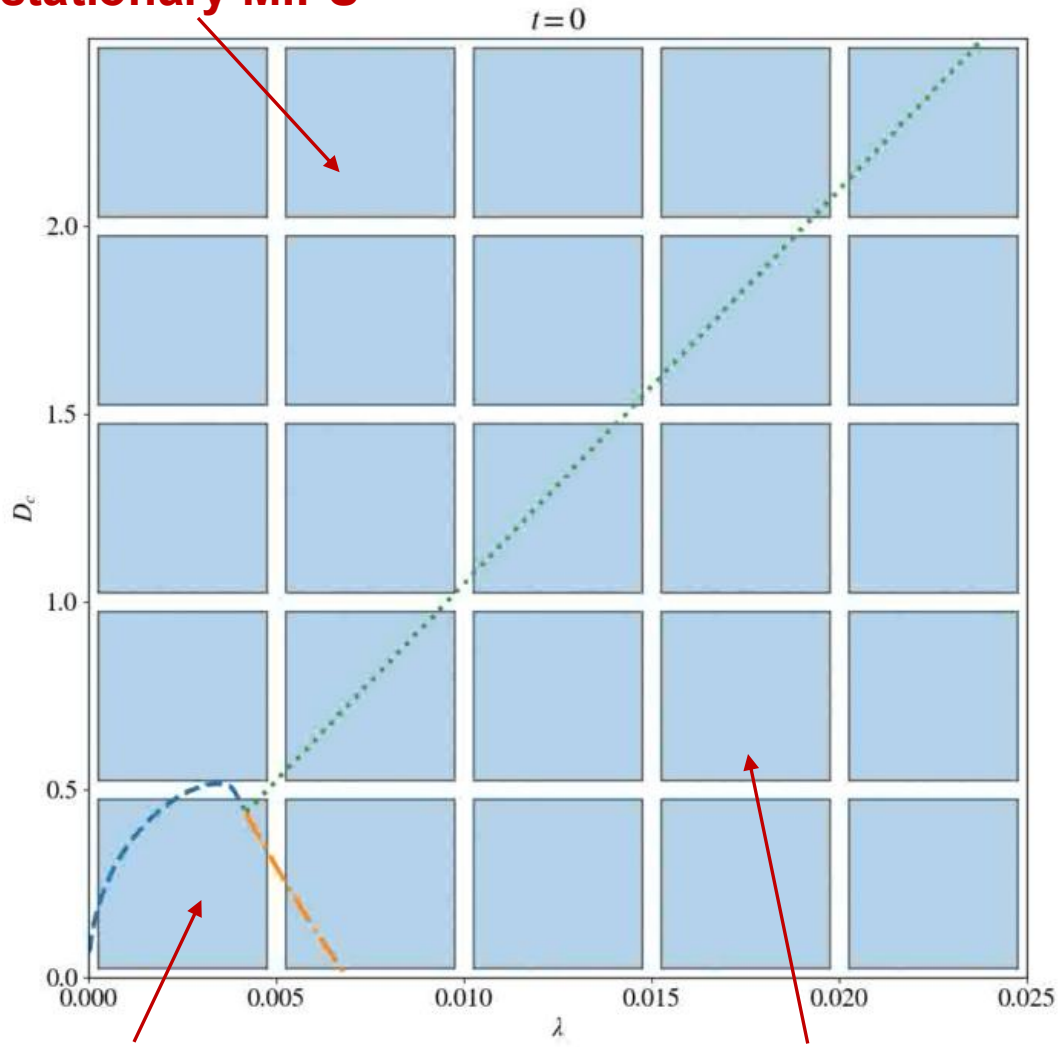


- MIPS region of the phase diagram is **narrower** compared to the vanilla MIPS.

- Cluster growth is **suppressed** than vanilla MIPS.

AMR phase diagram

- **AMR** (active metabolic regime)

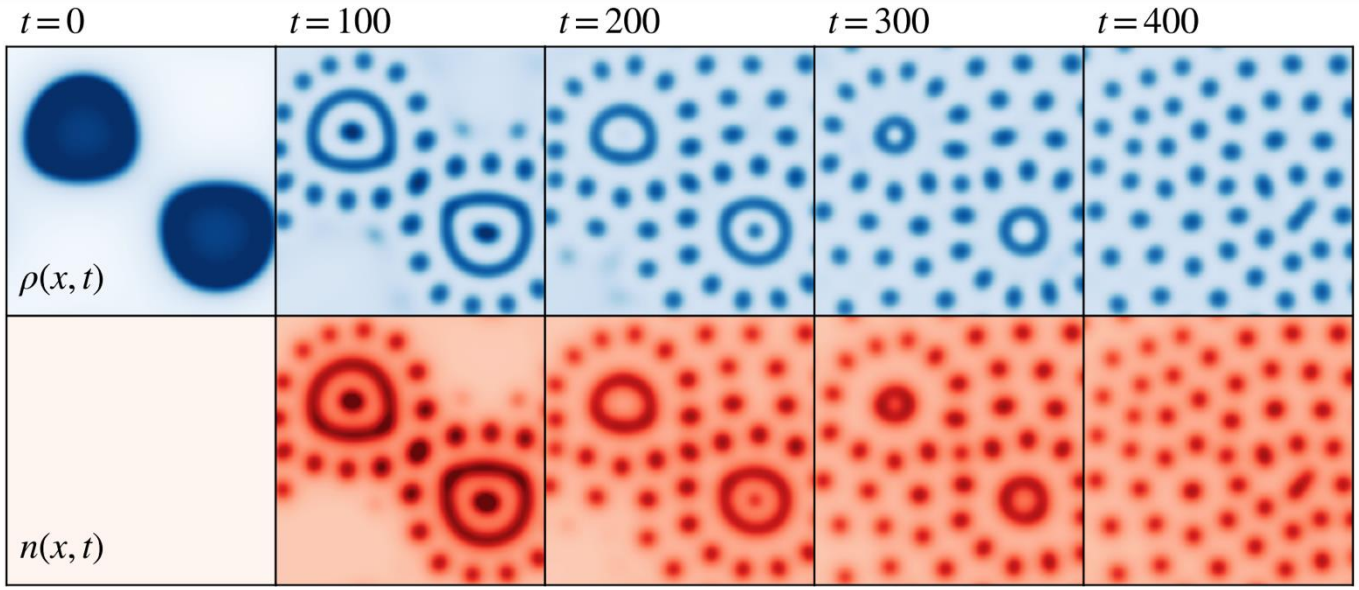


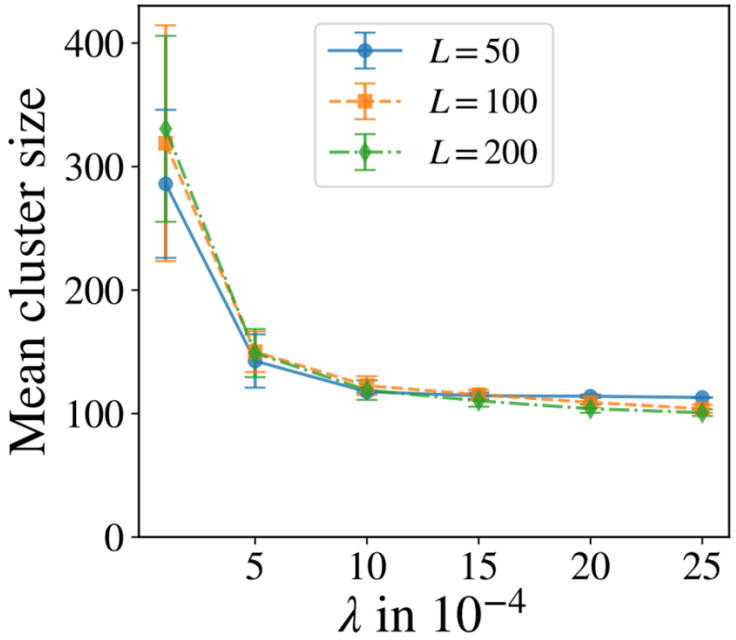
$$\dot{n}(\mathbf{r},t) = D_c\,\nabla^2 n + I\; - \lambda\rho\; v(\rho,n)\; n$$

- λ: coefficient of fuel consumption rate
- D_c: diffusion coefficient of fuel

AMR leads to microphase separation

- **AMR** (active metabolic regime) - further observation on Stationary MIPS phase

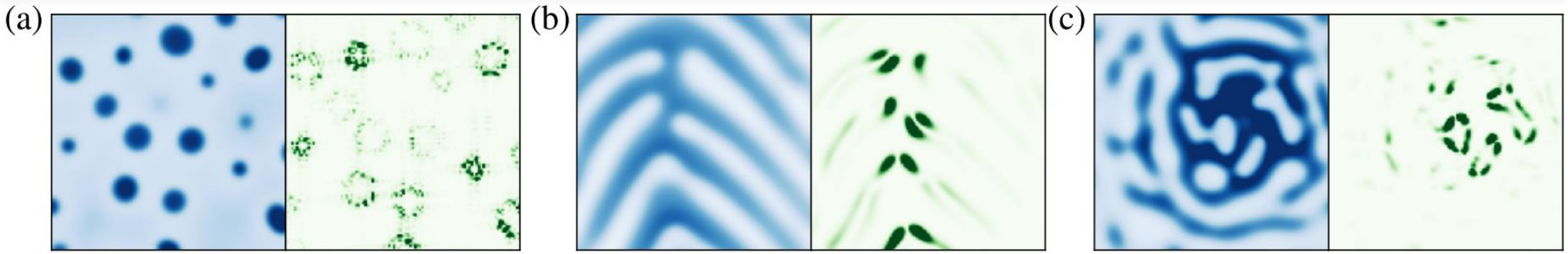




→ evidence of **microphase separation**

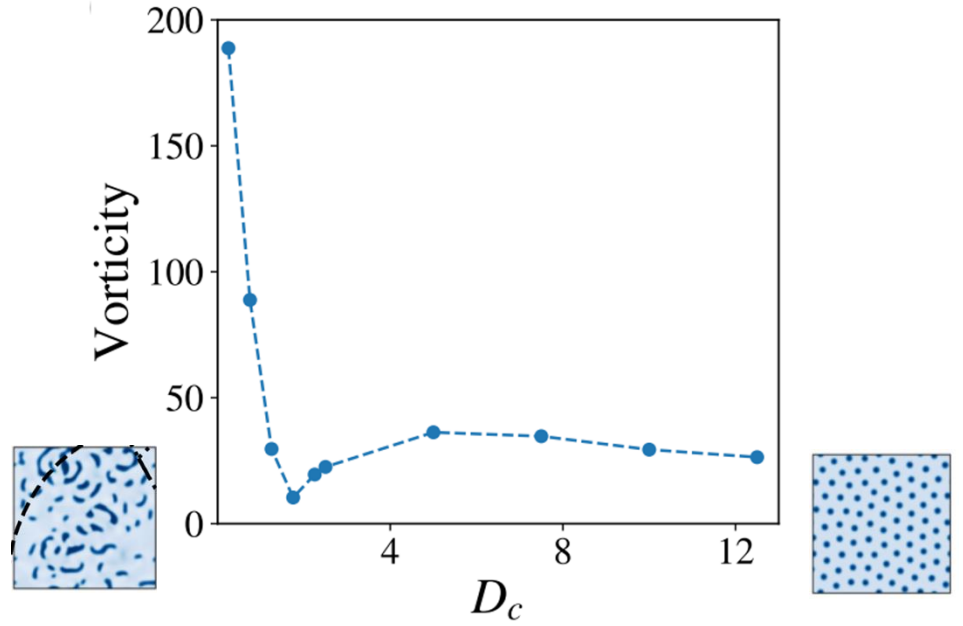
Quantifying the oscillatory phase

- **AMR** (active metabolic regime) - measure of **vorticity** for identifying the oscillatory phase



$$(\text{Vorticity}) = \frac{1}{L^2}\int d^2\boldsymbol{r}\left|\boldsymbol{\nabla}\times\frac{\boldsymbol{j}}{\rho}(\boldsymbol{r})\right|^2$$

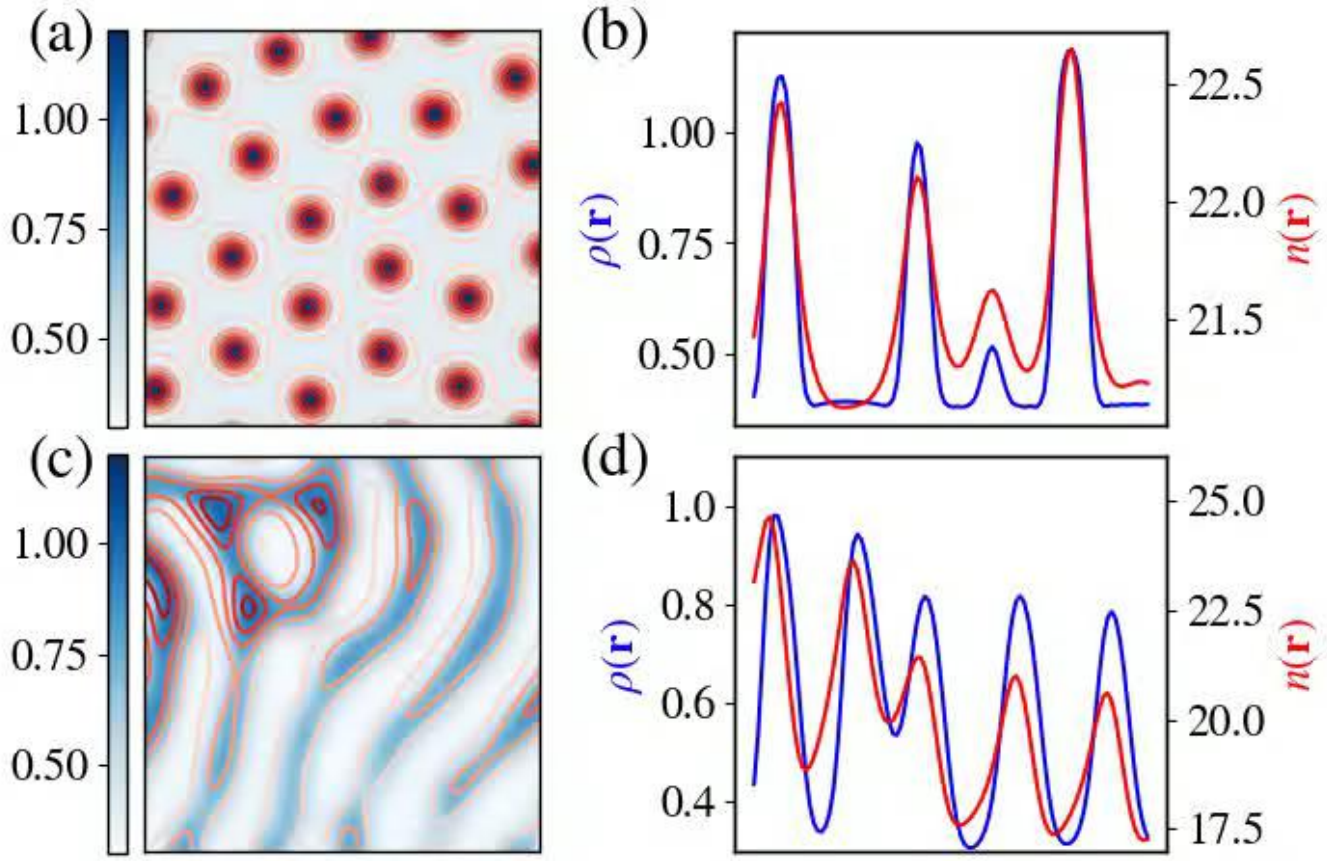
(j: probability current of the system)



oscillatory

stationary

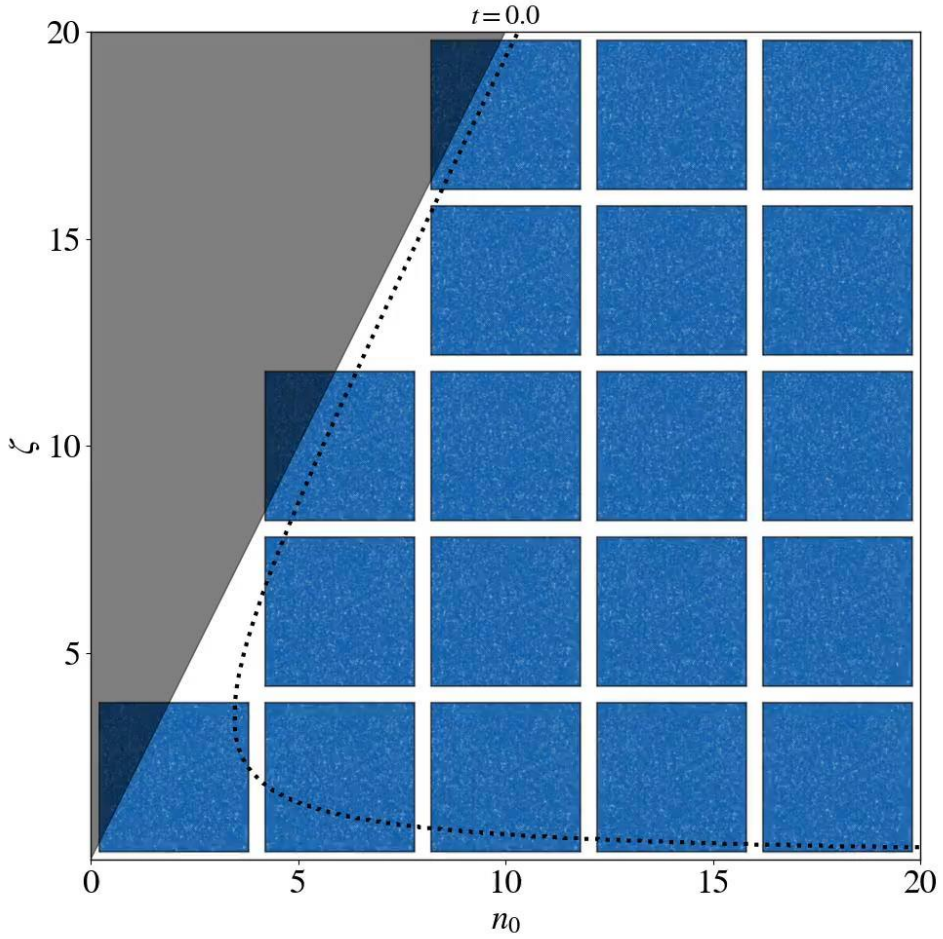
What causes the oscillation?



- There is nonreciprocal coupling between density and concentration fluctuations
- When the time scale of chemical relaxation is not too short, waves can be created by symmetry breaking

Particle-based models (quorum sensing)

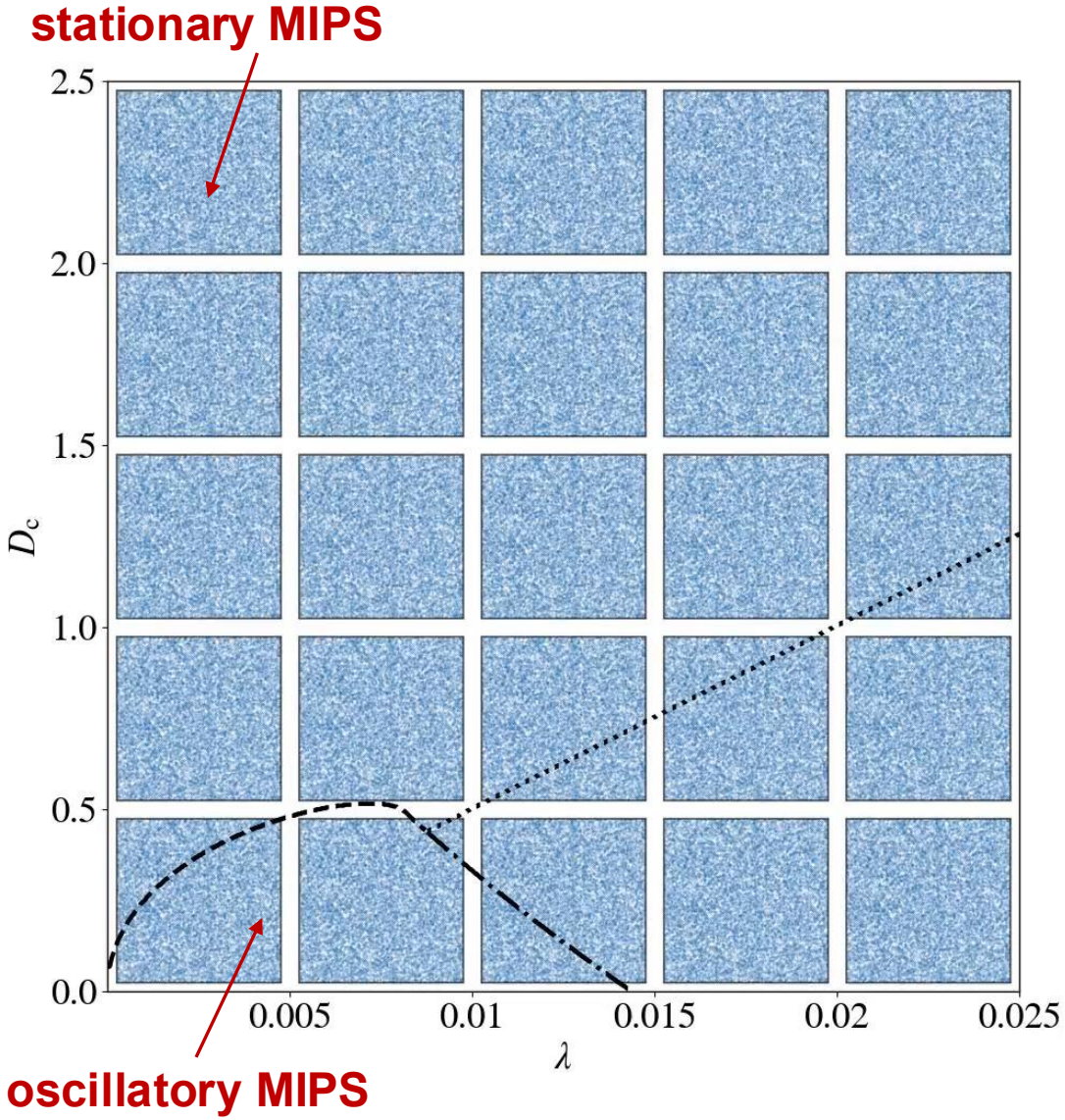
- **BMR** (basal metabolic regime)



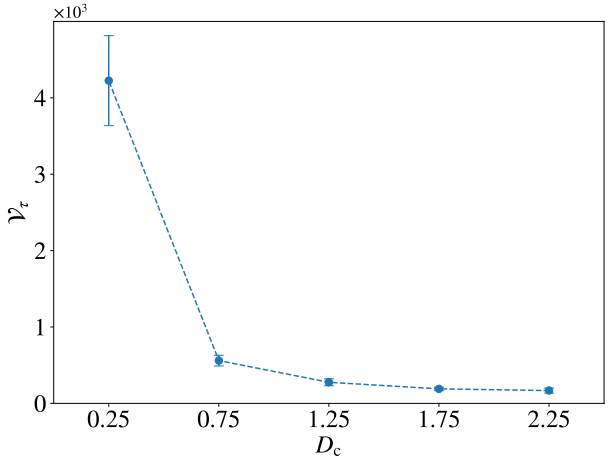
- Homogeneous and stationary phases observed
- Phase boundary is correctly predicted by the hydrodynamic theory
- Phase-separated patterns coarsen via the Ostwald process, eventually forming a single large-scale cluster

Particle-based models (quorum sensing)

- **AMR** (active metabolic regime)



- Homogeneous, stationary, and oscillatory phases are observed
- Stationary and oscillatory phases can be qualitatively distinguished by observing the time variability of density distribution



Conclusion and discussions

E. Kwon, Y. Oh, & YB
Commun. Phys. **8**, 288 (2025)

- We investigate how the changes in the self-propulsion strength via chemokinesis combined with chemical consumption affect the MIPS phenomenology of active particle.

- In the BMR, where the fuel consumption rate is proportional to the active particle density, the MIPS is always strengthened, leading to large-scale clusters.

- In the AMR, where the fuel consumption rate is proportional to the actual distances traveled by active particles, the MIPS is always suppressed, with microphase separation and oscillatory patterns.

- The hydrodynamic model and the particle-based model exhibit some degree of agreement, but the oscillatory patterns predicted by the former may not be stable against the effects of noises or higher-order terms.