Complex Disordered Systems

Active Matter

Francesco Turci

Today

- Beyond thermal equilibrium
- Run-and-tumble dynamics
- Active Brownian particles
- Motility-induced phase separation (MIPS)

Beyond Thermal Systems

Equilibrium systems systems:

- Free energy is optimised (subject to constraints):
- Distribution of states given by Boltzmann statistics:

$$P(\mathrm{state}) \propto e^{-E(\mathrm{state})/k_B T}$$

Arrested systems

- Supercooled liquids: local equilibrium (thermal)
- Glasses/gels: slow relaxation (towards equilibrium)

Active matter: Nonequilibrium via **local dissipation**

- Local energy consumption
- Self-propulsion
- Dissipation at microscopic scale

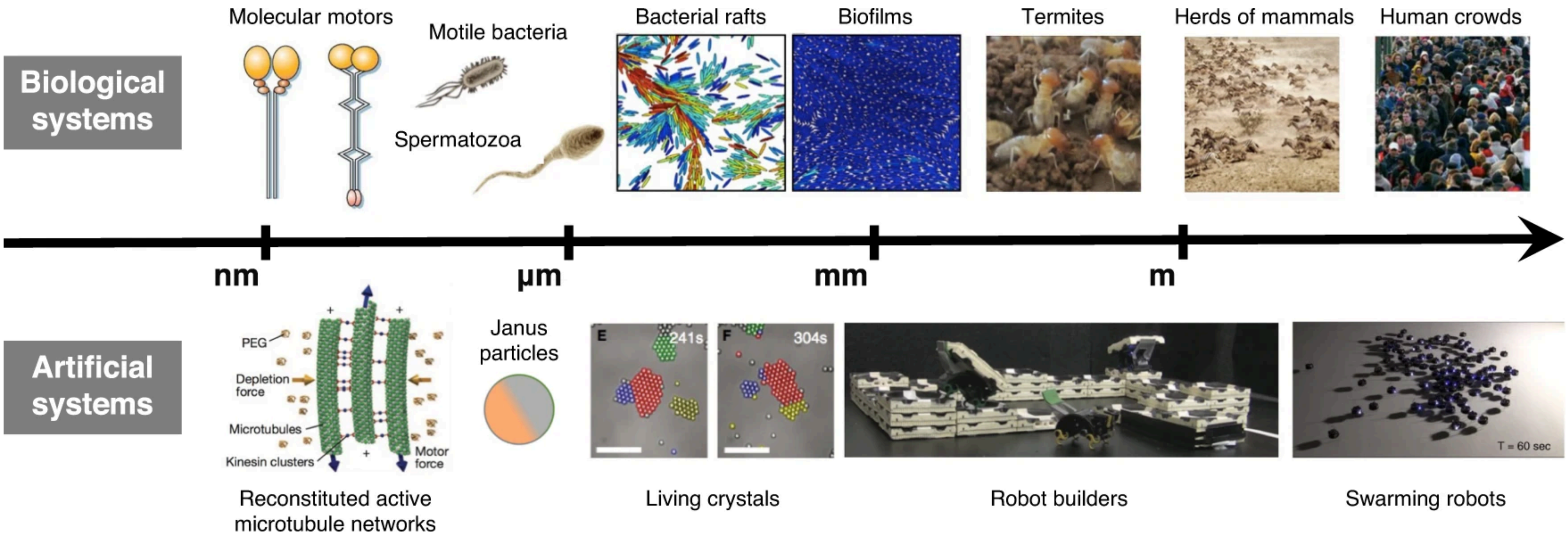
Examples:

- Bacteria
- Synthetic microswimmers
- Molecular motors
- Bird flocks, fish schools

> In a active systems, the distribution of states is **not given** by Boltzmann statistics!

Examples of Active Matter

Some examples



Flocking as a minimal model

Flocking as a minimal model

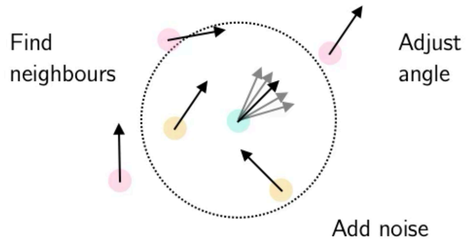
The **Vicsek model** (1995) was one of the simplest models of active matter. Key ingredients: **alignment + self propulsion**

- N particles with positions $\mathbf{r}_i$ and orientations θ_i
- Update rules:

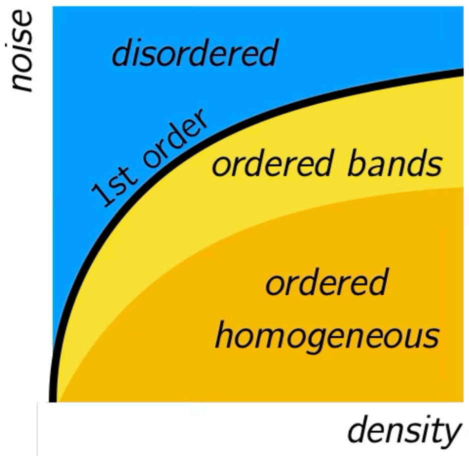
$$\mathbf{r}_i(t+1) = \mathbf{r}_i(t) + v_0 \hat{\mathbf{n}}_i(t)$$

$$\theta_i(t+1) = \langle \theta_j \rangle_{|\mathbf{r}_j - \mathbf{r}_i| < R} + \eta_i$$

- v_0: constant speed
- R: interaction radius
- η_i: noise term (uniform random in $[-\pi/2, \pi/2]$)



Vicsek et al, PRL 1995



Chaté et al PRL 2004

Flocking as a minimal model

Vicsek simulation

Run-and-Tumble Motion

Further inspirations from the microbial world, where dissipation can be more directly observed (and even tuned).

Inspired by bacterial motion (*E. coli*)

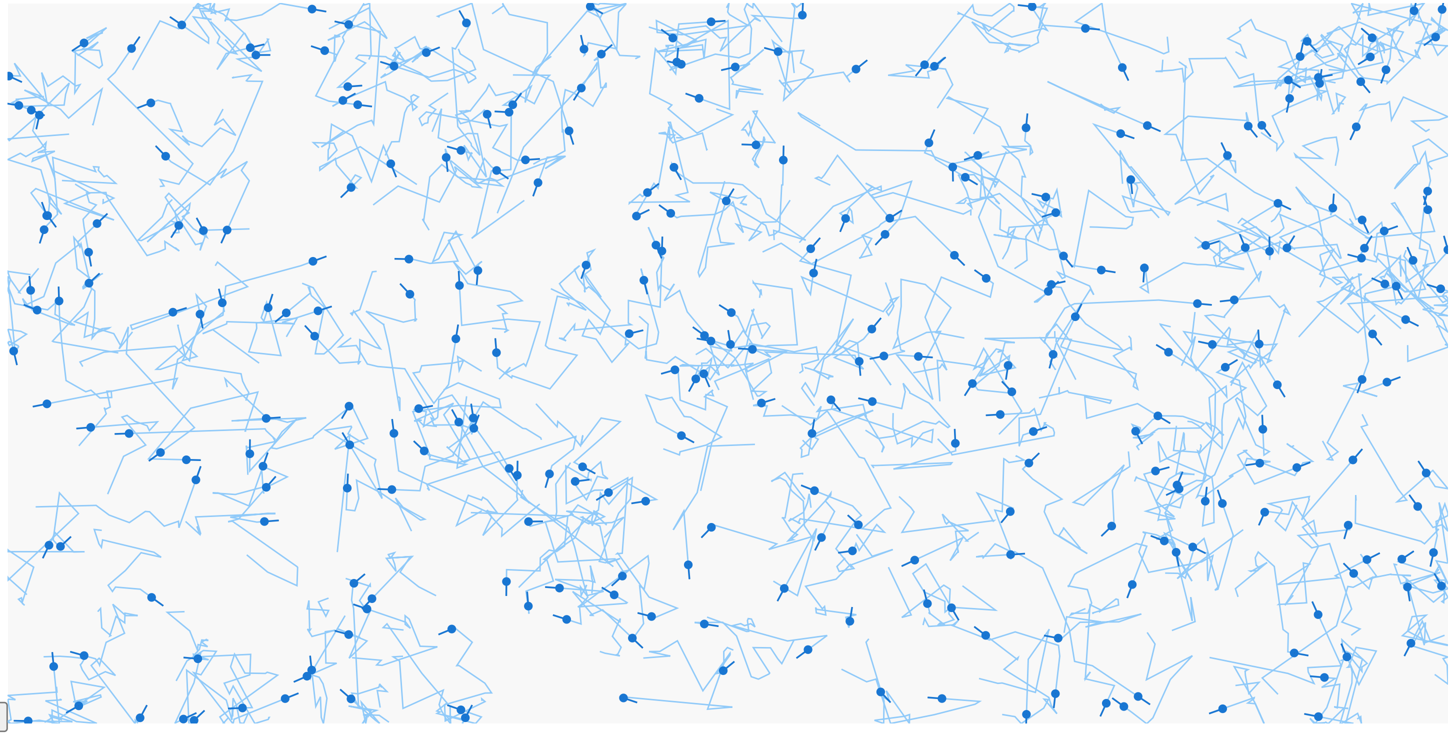
Two phases:

- **Run**: Straight-line motion at constant speed v_0
- **Tumble**: Random reorientation

Key parameter: Tumble rate λ

Run-and-Tumble: Dynamics

Tumble rate λ 0.1



Pause

Figure 1: Non-interacting run and tumble particles.

Run-and-Tumble dynamics

Run phase (constant velocity):

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + v_0 \hat{\mathbf{n}}(t) \Delta t$$

Tumble phase (random reorientation):

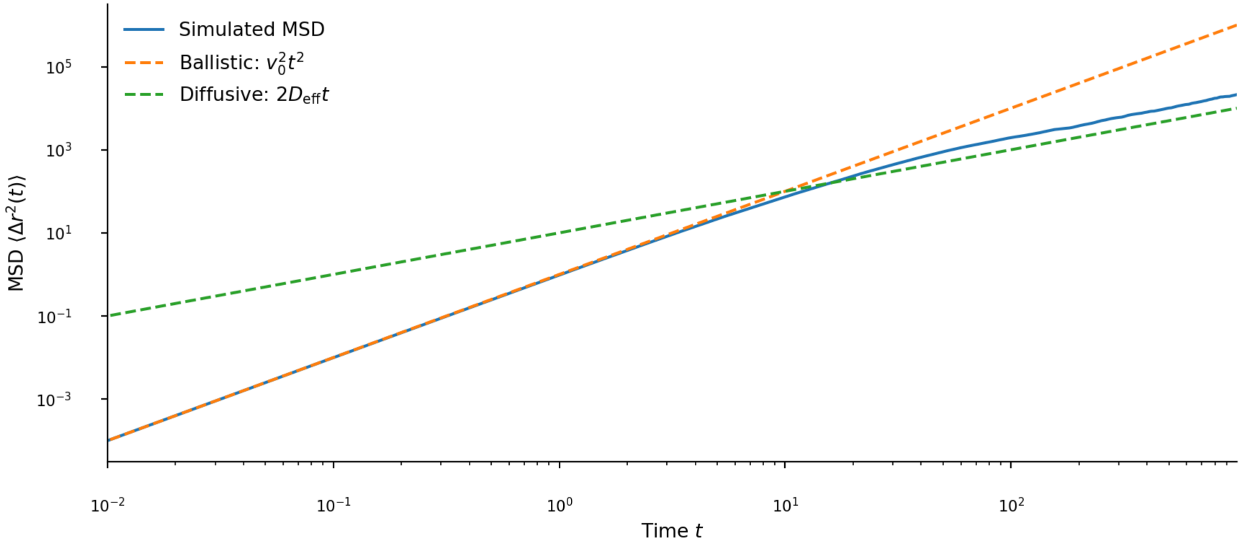
- With probability $\lambda \Delta t$: randomize $\hat{\mathbf{n}}$
- Otherwise: continue running

Mean Squared Displacement

Two regimes

1. **Ballistic** (short times): $\langle \Delta r^2(t) \rangle \sim v_0^2 t^2$
2. **Diffusive** (long times, $t \gg 1/\lambda$): $\langle \Delta r^2(t) \rangle \sim 2D_{\mathrm{eff}} t$
   - Effective diffusion: $D_{\mathrm{eff}} = \frac{v_0^2}{2\lambda}$ (2D)

Crossover time: $t_c \sim 1/\lambda$



Active Brownian Particles (ABPs)

Minimal model for self-propelled colloids (e.g., Janus particles)

Dynamics:

- Translational motion

$$\frac{d\mathbf{r}}{dt} = v_0\hat{\mathbf{n}}(t) + \sqrt{2D_t}\boldsymbol{\xi}(t)$$

- Rotational motion

$$\frac{d\theta}{dt} = \sqrt{2D_r}\eta(t)$$

- v_0: self-propulsion speed
- D_t: translational diffusion
- D_r: rotational diffusion
- Continuous reorientation

Péclet Number:

$$Pe = \frac{v_0}{\sqrt{D_t D_r}} = \frac{v_0}{D_r L}$$

- Measures activity strength vs thermal motion
- $Pe \ll 1$: thermal equilibrium limit
- $Pe \gg 1$: strong activity, far from equilibrium
- $L = \sqrt{D_t/D_r}$: characteristic length scale

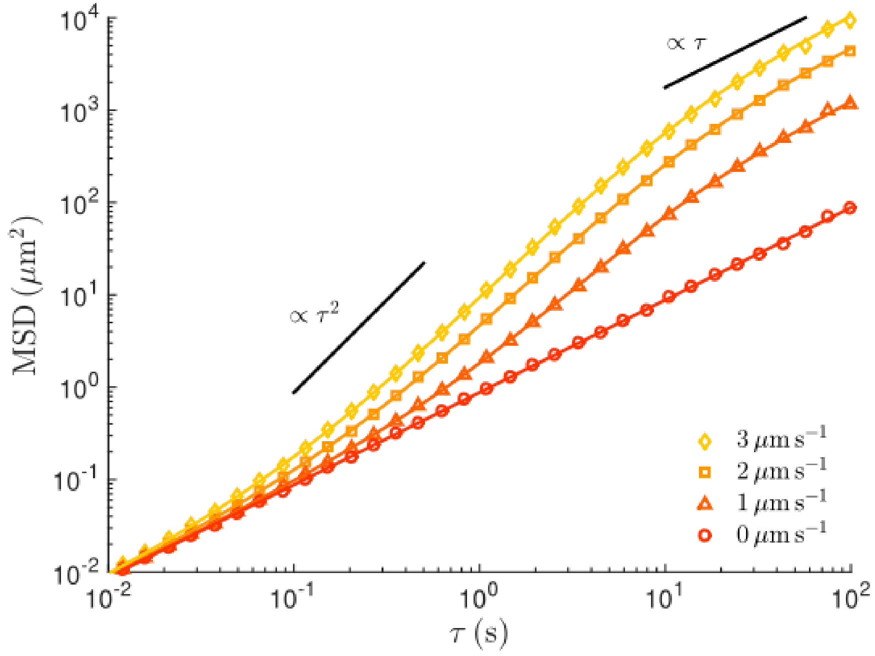
ABP: Mean Squared Displacement

Three regimes:

$$\langle \Delta r^2(\tau) \rangle = \left[4D_T + 2v^2\tau_R\right]\tau + 2v^2\tau_R^2\left(e^{-\tau/\tau_R} - 1\right)$$

1. **Short times**: Diffusive $\sim 4D_T\tau$
2. **Intermediate**: Ballistic $\sim v_0^2\tau^2$
3. **Long times**: Enhanced diffusion

- $\tau_R = 1/D_r$: persistence time
- $D_{\text{eff}} = \frac{v_0^2}{2D_r}$: effective diffusion

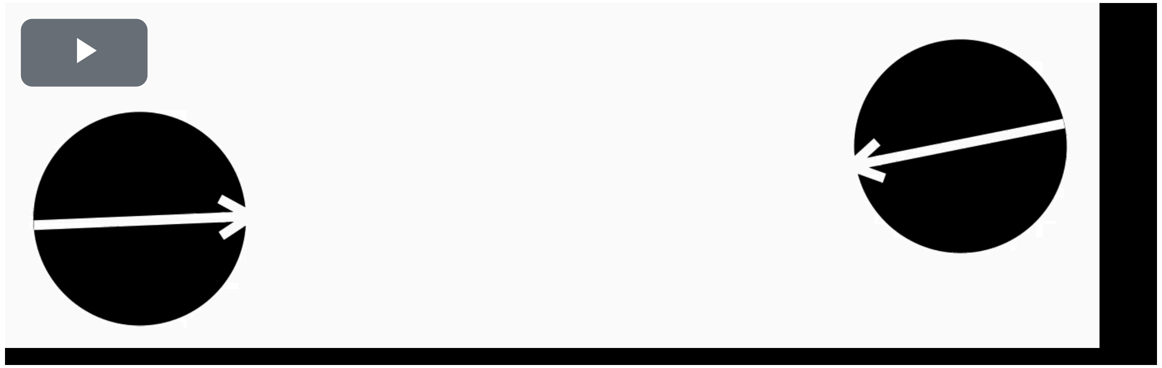


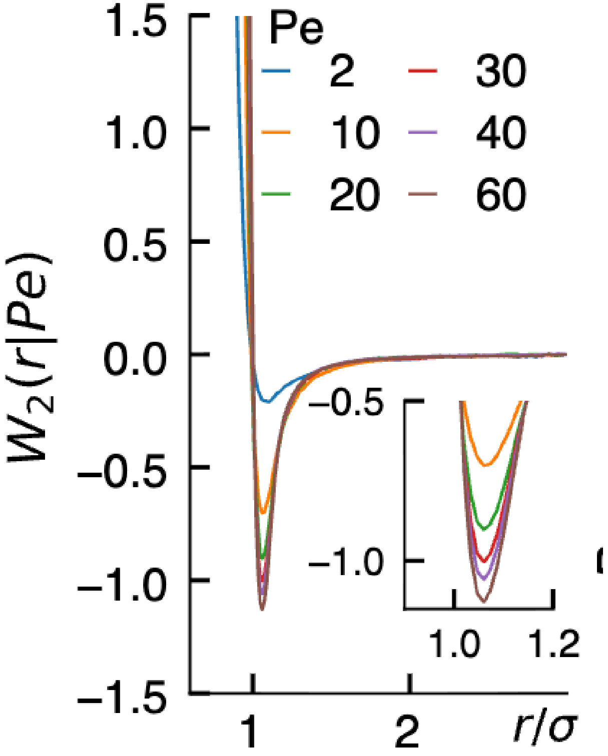
Mean squared displacement for ABPs at different self-propulsion speeds.

Effective Interactions

The persistence of active motion can lead to effective interactions between particles.

- Head-to-head collisions lead to a persistence time of contact between two particles
- This can be seen as an effective attraction between particles



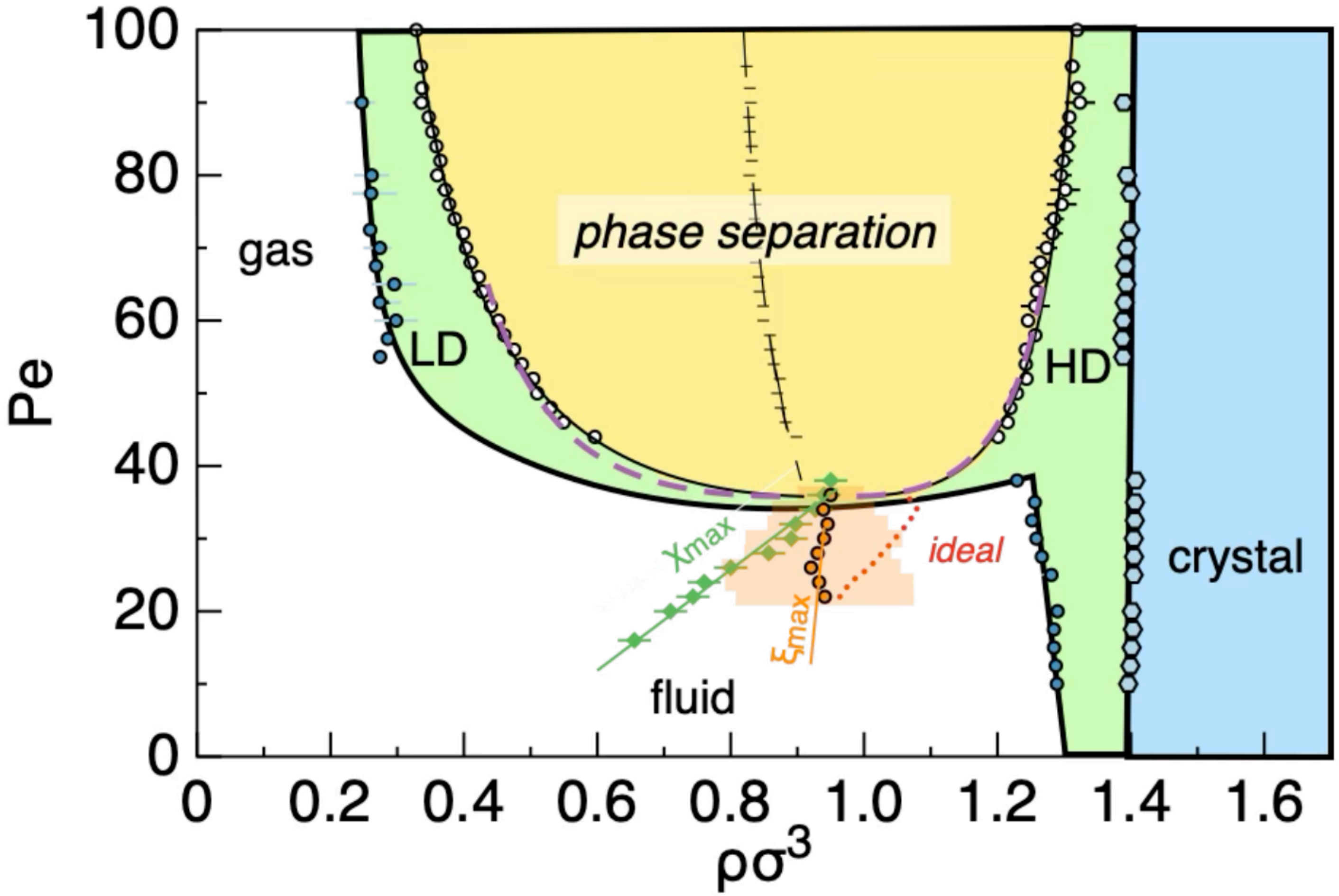


Effective twobody potential for ABPs, Turci & wilding PRl 2021

(The realiity is more complex, with many-body effects!)

Motility-Induced Phase Separation (MIPS)

Interacting ABPs → nonequilibrium self-organization



MIPS in 3D ABPs from Turci and Wilding Physical Review Letters 2021

Key idea: Purely repulsive particles (hard spheres) + ABP dynamics

MIPS Mechanism

Equilibrium (no self-propulsion):

- Hard spheres
- No liquid-gas separation

Active (with self-propulsion):

- Head-to-head collisions
- Finite residence time
- Many-body caging
- Density heterogeneities

As D_r decreases:

- More persistent motion
- System more out-of-equilibrium
- Enhanced density fluctuations
- **Spontaneous phase separation**

MIPS: Critical-like Behavior

Phase diagram features:

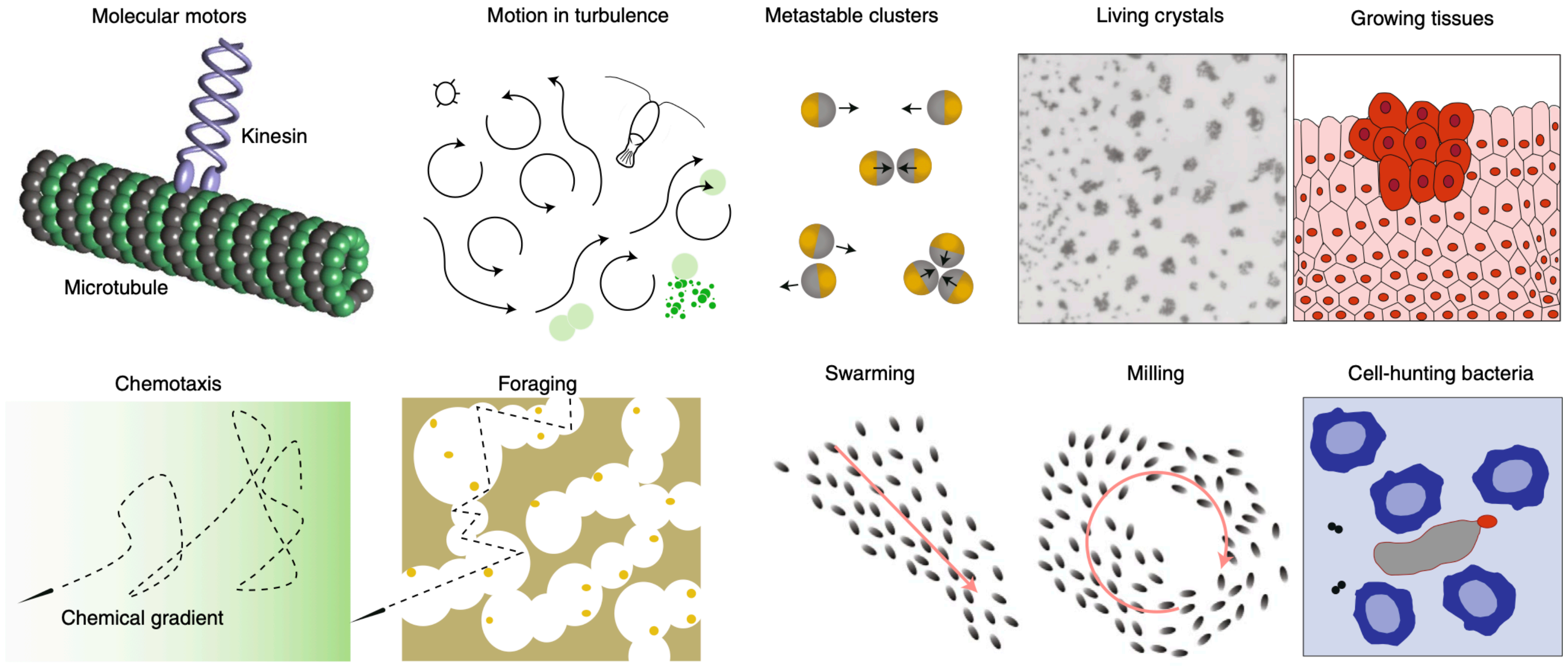
- **Low** D_r: Dense + dilute phases (like liquid-gas)
- **Critical point**: Enhanced fluctuations
- MIPS exists both in 2d and 3D:
  - in 2D, disk ordering at high densities
  - in 3D, MIPS is **metastable** to gas-crystal, like colloid polymer mixtures.
- **Short-range effective interactions** between active particles

Result: Nonequilibrium phase transition in purely repulsive system!

Experimental realisation of active matter

In experiments, active systems can be realised in various ways:

- **Bacterial suspensions**: e.g., *E. coli*, *B. subtilis*
- **Synthetic microswimmers**: Janus particles with catalytic coatings
- **Light-activated colloids**: Particles that change motility under light
- **Vibrated granular matter**: Macroscopic particles on vibrating plates
- **Nano- and micro-robots**: Swarms of tiny robots with programmed motion



Experimental systems and active. matter behaviours