Active dumbbells

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Work in collaboration with

D. Loi & S. Mossa (Grenoble, France, 2007-2009) and

G. Gonnella, P. Di Gregorio, G.-L. Laghezza, A. Lamura, A. Mossa & A. Suma

(Bari & Trieste, Italia, 2013-2015)

Palma de Mallorca, España, 2017

Plan

5 lectures & 2 exercise sessions

1. Introduction
2. Active Brownian dumbbells
3. Effective temperatures
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

First lecture

Plan

5 lectures & 2 exercise sessions

1. **Introduction**
2. Active Brownian dumbbells
3. Effective temperatures
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

Introduction

General setting

- Closed & open systems
- Equilibrium & out of equilibrium
  - Long time scales
  - Forces & energy injection
- Individual & collective effects
- Three dimensions *vs.* two dimensions

Introduction

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Isolated systems

Dynamics of a classical isolated system

Foundations of statistical physics.

Question : does the dynamics of a particular system reach a flat distribution over the constant energy surface in phase space ?

Ergodic theory, $\in$ mathematical physics at present.

Dynamics of a (quantum) isolated system :

a problem of current interest, recently boosted by cold atom experiments.

Question : after a quench, i.e. a rapid variation of a parameter in the system, are at least some observables described by thermal ones ? When, how, which ?

we shall not discuss these issues here

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- **Three dimensions** *vs.* **two dimensions**

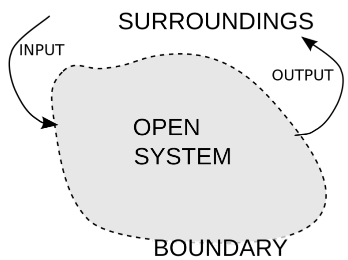
Open systems

Aim

Our interest is to describe the statics and dynamics of a classical (or quantum) system coupled to a classical (or quantum) environment.

The Hamiltonian of the ensemble is

$$\boxed{H = H_{syst} + H_{env} + H_{int}}$$



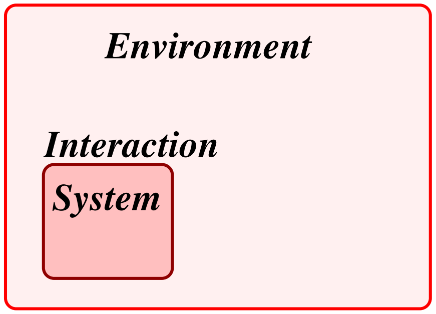
The dynamics of all variables are given by Newton (or Heisenberg) rules, depending on the variables being classical (or quantum).

The total energy is conserved, $E =$ ct but each contribution is not, in particular, $E_{syst} \neq$ ct, and we'll take $e_0 \ll E_{syst} \ll E_{env}$.

Dynamics in equilibrium

Conditions

Take an open system coupled to an environment



Necessary :

— The bath should be in equilibrium

same origin of noise and friction.

— Deterministic force :

conservative forces only, $\vec{F} = -\vec{\nabla} V$.

— Either the initial condition is taken from the equilibrium pdf, or the latter should be reached after an equilibration time t_{eq} :

$$P_{eq}(v, x) \propto e^{-\beta(\frac{mv^2}{2} + V)}$$

What do we know ?

Equilibrium collective phenomena

$N \gg 1$ collective phenomena lead to phase transitions.

E.g., gas, liquid, solid phase transitions in molecular systems.

We understand the nature of the equilibrium phases and the phase transitions. We can describe the phases with mean-field theory and the critical behaviour with the renormalization group.

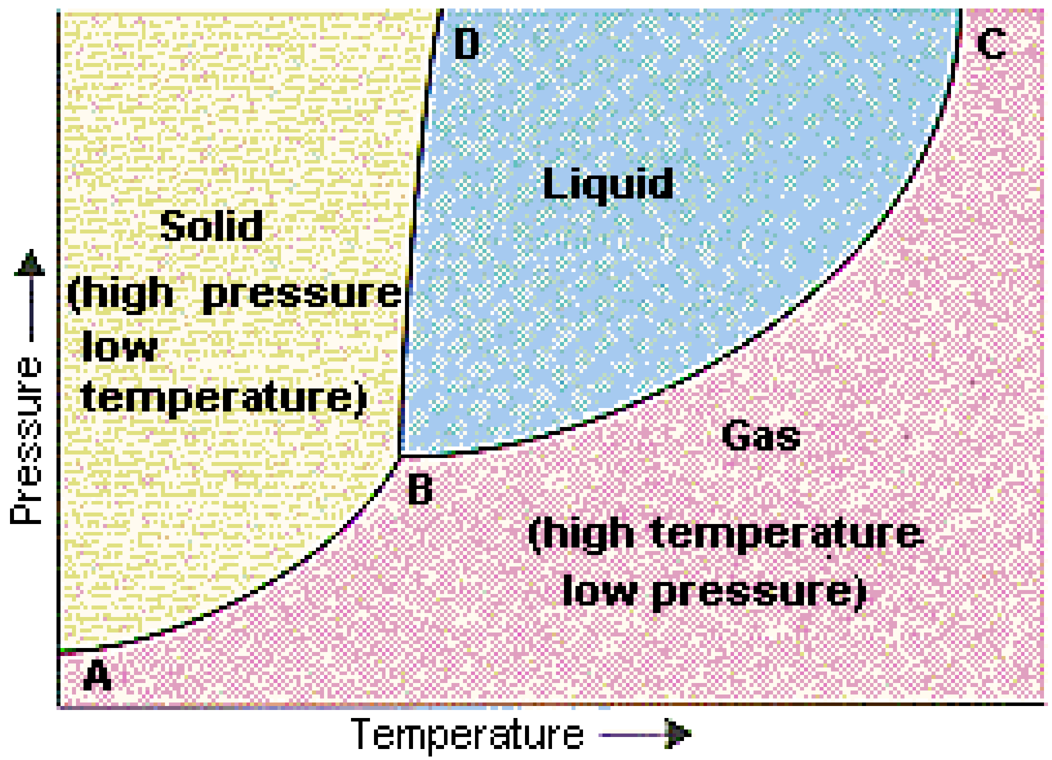
Quantum and thermal fluctuations conspire against the ordered phases.

We understand the equilibrium and out of equilibrium relaxation at the critical point or within the phases. We typically describe it with the dynamic RG at the critical point or the dynamic scaling hypothesis in the ordered phase.

E.g., growth of critical structures or ordered domains.

What do we know ?

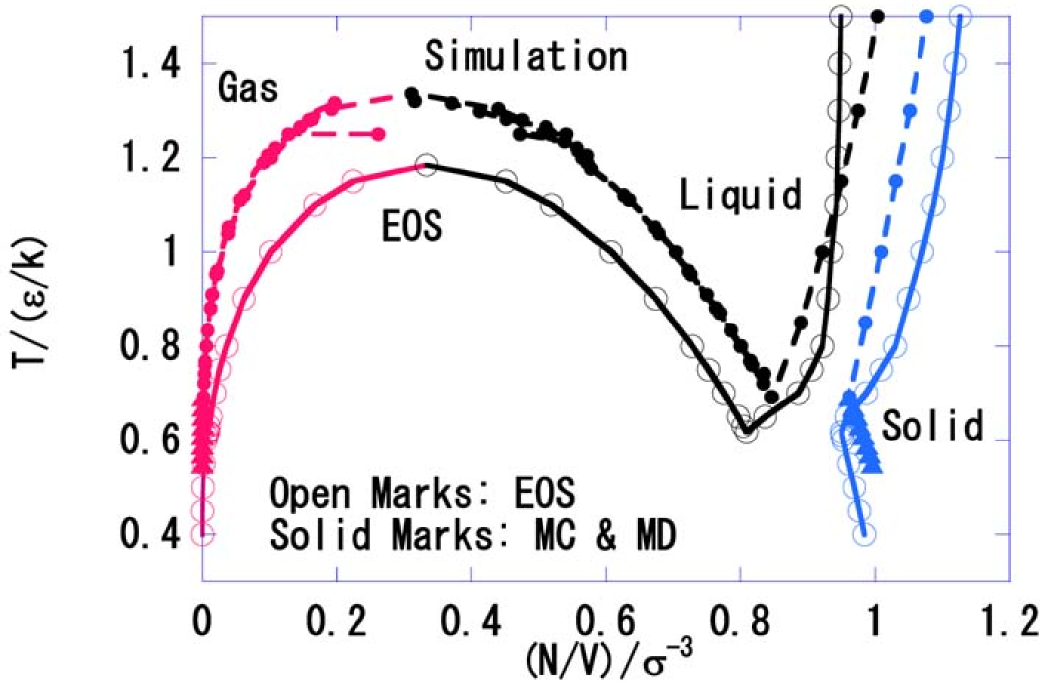
Solid, liquid and gas equilibrium phases



Typical (simple) (P, T) phase diagram

What do we know ?

Solid, liquid and gas equilibrium phases



Typical (simple) (ϕ, T) phase diagram

Lennard-Jones model system for Argon (more later)

Kataoka & Yamada, J. Comp. Chem. Jpn. 11, 81 (2012)

Equilibrium phases

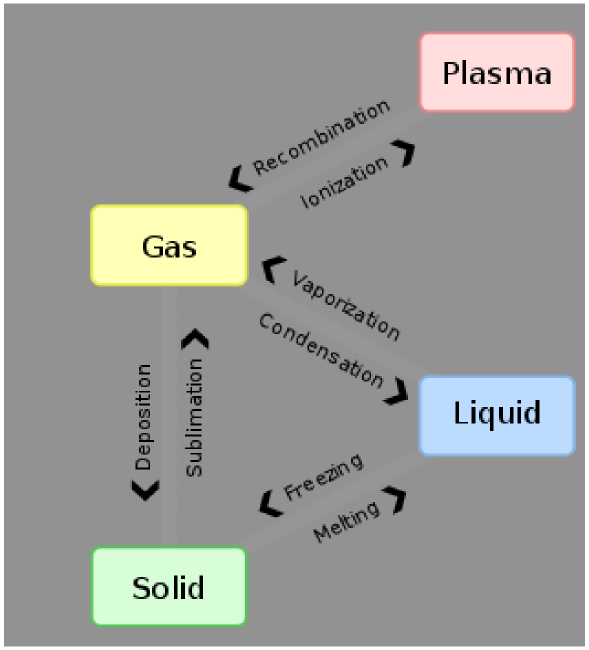
Macroscopic properties

- A gas is an an air-like fluid substance which expands freely to fill any space available, irrespective of its quantity.
- A liquid is a substance that flows freely but is of constant volume, having a consistency like that of water or oil. It takes the shape of its container
- A solid is a material with non-vanishing shear modulus.
- A crystal is a system with long-range positional order.

  It has a periodic structure and its ‘particles’ are located close to the nodes of a lattice.

Phases and transitions

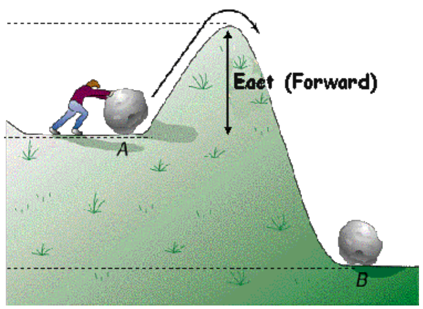
Names

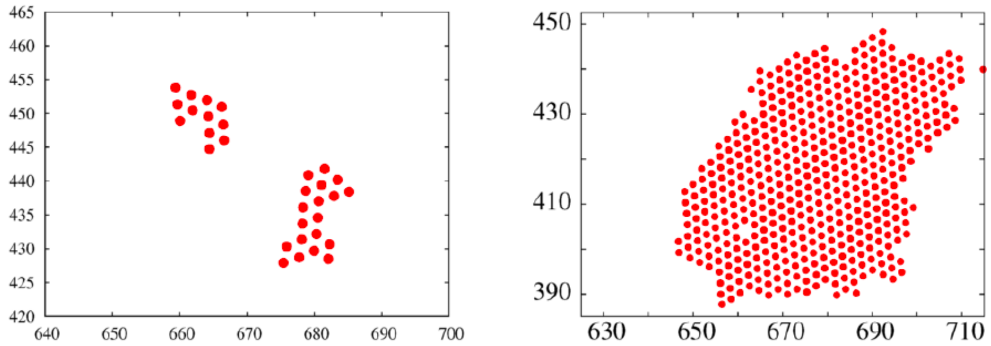


The states of matter have uniform physical properties in each phase. During a phase transition certain properties change, often discontinuously, as a result of the change of an external condition, such as temperature, pressure, or others.

Freezing transition

From liquid to solid : nucleation & growth





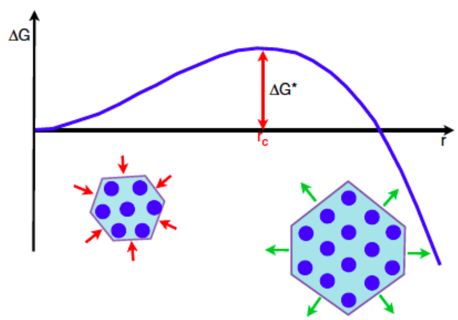
Nucleation barrier $\Delta F(r)$ Examples of two crystalline nuclei

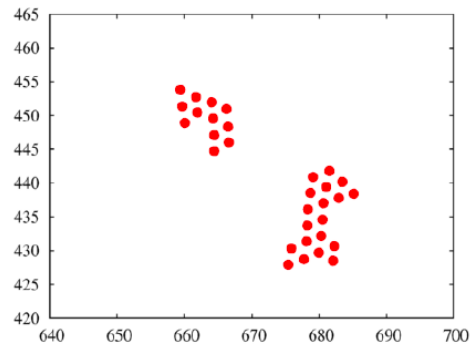
$2d$ order of attractive colloids forming a triangular lattice (more later)

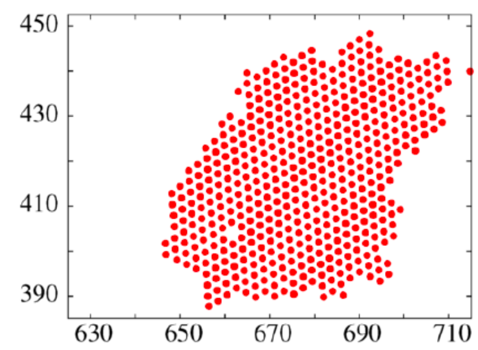
Images borrowed from **González, Crystals 6, 46 (2016)**

Freezing transition

From liquid to solid : nucleation & growth







Nucleation barrier $\Delta F(r)$

Examples of two crystalline nuclei

$2d$ order of attractive colloids forming a triangular lattice (more later)

Left image from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

Freezing transition

Different routes in $3d$ and $2d$

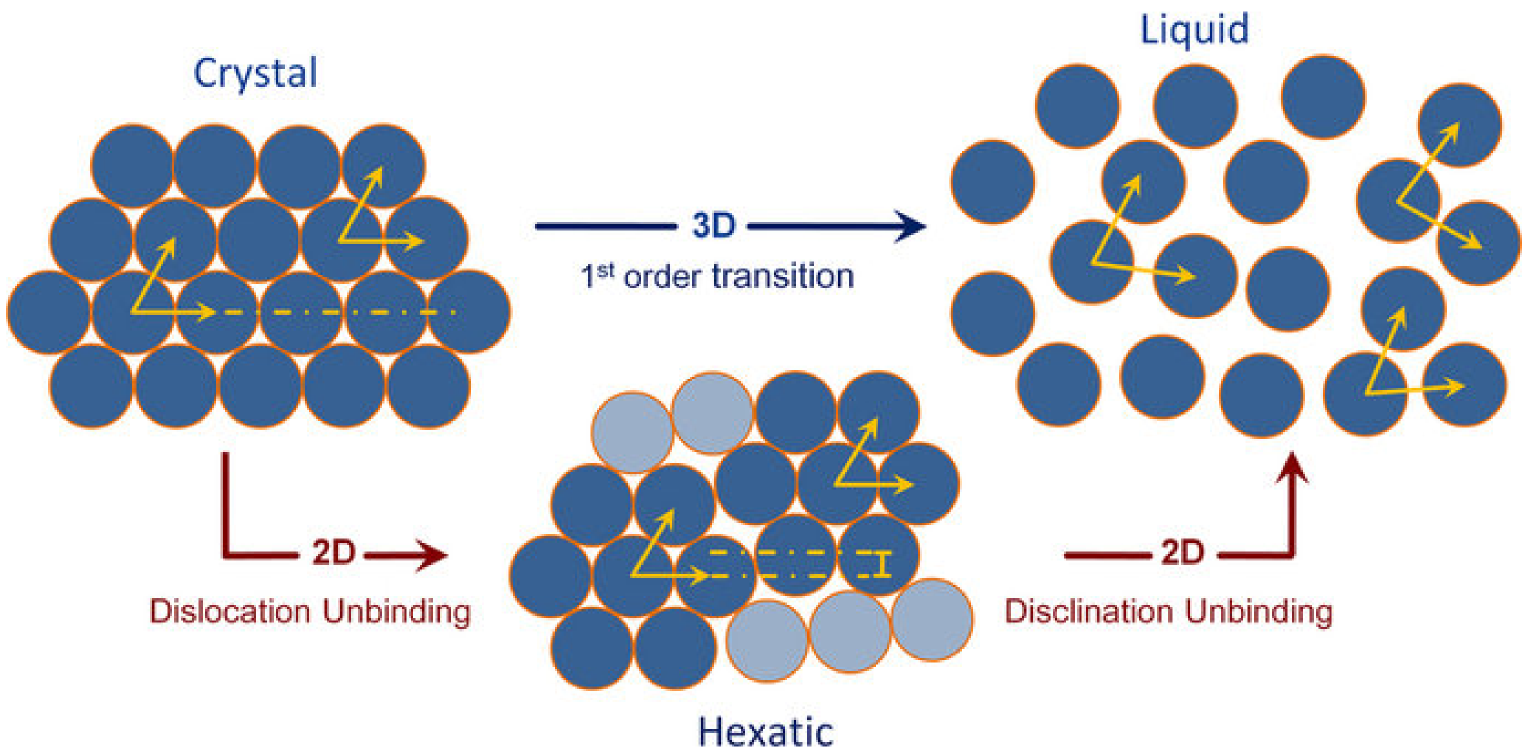


Image from **Pal, Kamal & Raghunathan, Sc. Rep. 6, 32313 (2016)**

Solids

$3d$ vs. $2d$

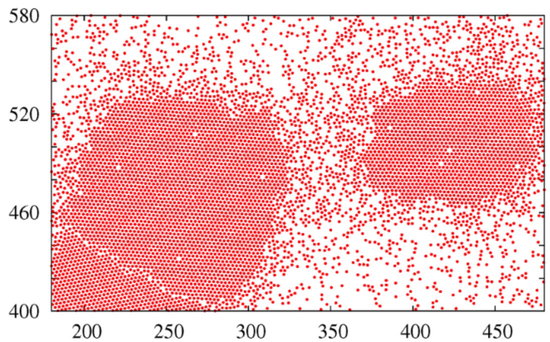
- A solid is a material with non-vanishing shear modulus.
- A crystal is a system with long-range positional order.

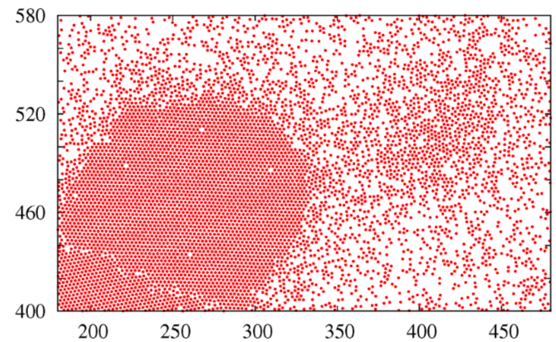
  It has a periodic structure and its ‘particles’ are located close to the nodes of a lattice.

  The position fluctuations are bounded $\Delta^2 = \langle(\boldsymbol{r}_i - \boldsymbol{r}_i^{\rm latt})\rangle < \infty$
- $2d$ solids exist but have a weaker ordering than $3d$ ones.
  - They are oriented crystals with no positional order.
  - Critical phase with algebraic relaxation of position correlations.
  - Phase transition *à la* Kosterlitz-Thouless (Nobel Prize).

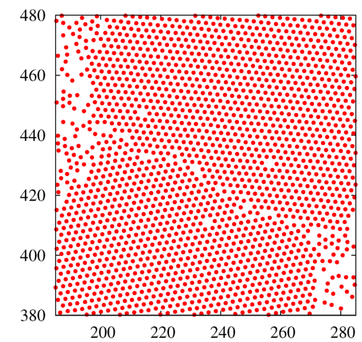
Freezing transition

$2d$ crystalline clusters & defects





Two clusters



Grain boundary

Images borrowed from **González, Crystals 6, 46 (2016)**

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What we do not know

Long time-scales for relaxation

Systems with competing interactions remain out of equilibrium and it is not clear

- whether there are phase transitions,
- which is the nature of the putative ordered phases,
- which is the dynamic mechanism.

Examples are :

- systems with quenched disorder,
- systems with geometric frustration,
- glasses of all kinds.

Static and dynamic mean-field theory has been developed – both classically and quantum mechanically – and they yield new concepts and predictions.

Extensions of the RG have been proposed and are currently being explored.

Glassy features

What do they have in common ?

— No obvious spatial order, disorder (differently from crystals).

— Many metastable states

Rugged landscape

— Slow non-equilibrium relaxation

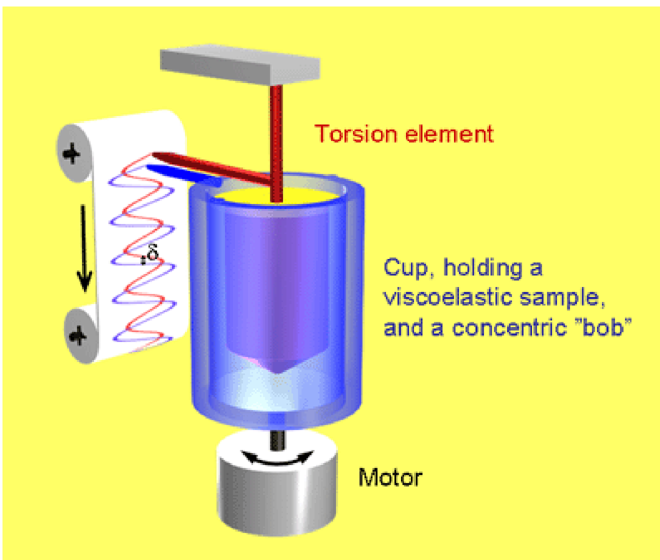
$$\boxed{\tau_{\rm micro} \lll \tau_{\rm exp} \lll \tau_{\rm relax}}$$

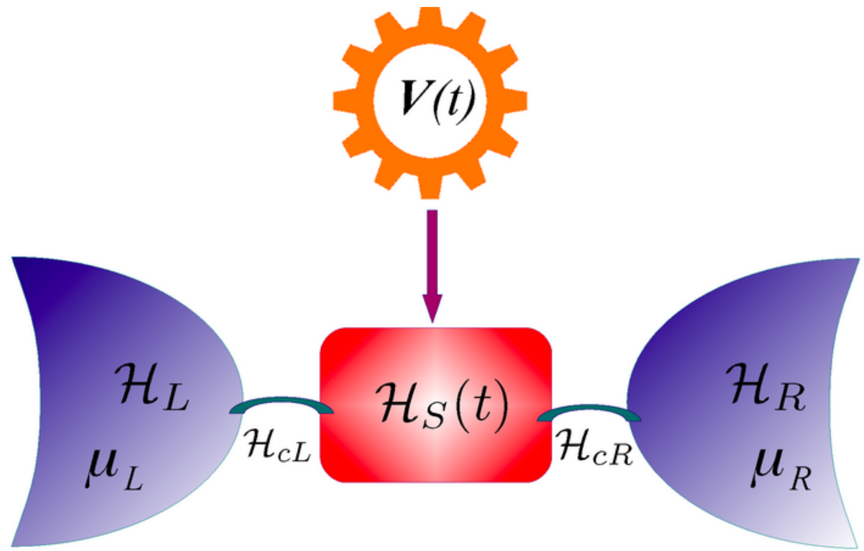
Time-scale separation

— Hard to make them flow under **external forces - energy injection**

Energy injection

Traditional : from the borders (outside)



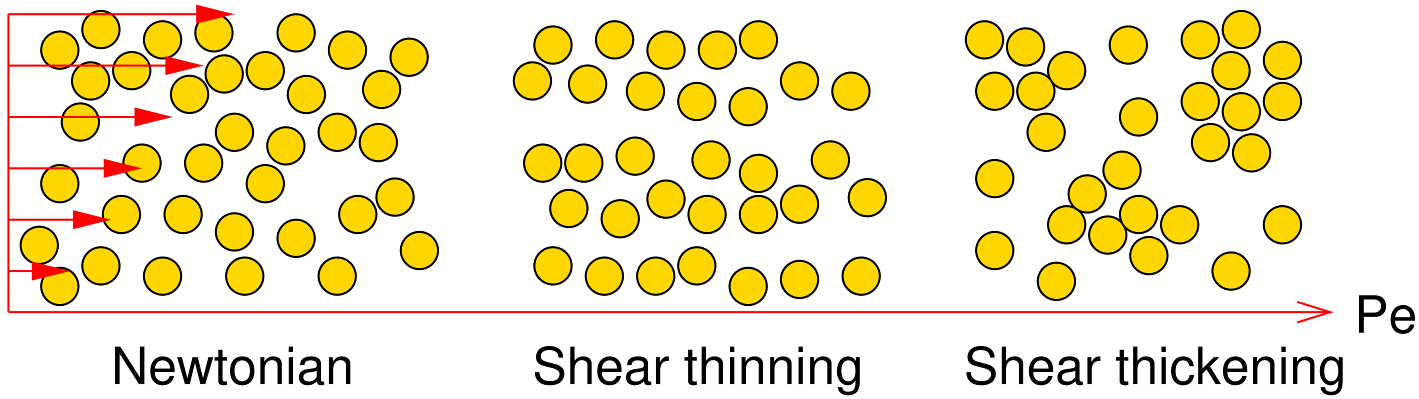


Rheology

Transport

Drive & transport

Rheology of complex fluids



Rheology of complex fluids

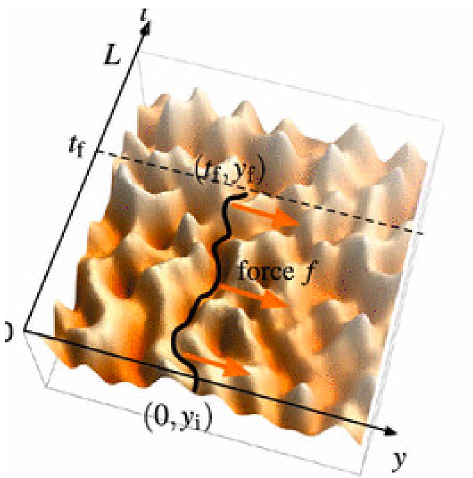
Shear thinning τ_{relax} decreases, *e.g.* paints

Shear thickening τ_{relax} increases, *e.g.* cornstarch & water mix

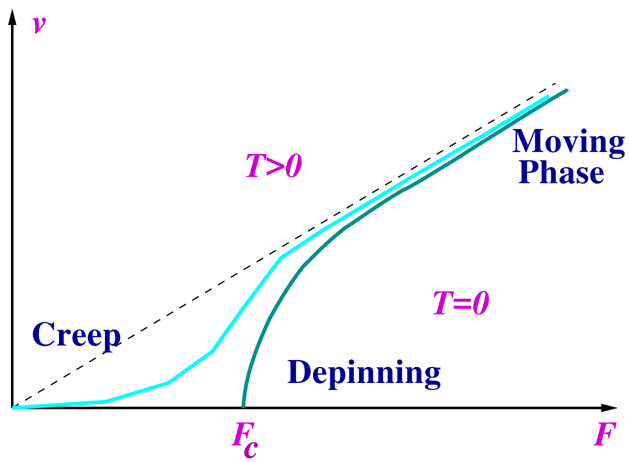
e.g. review **Brader 10**

Drive & transport

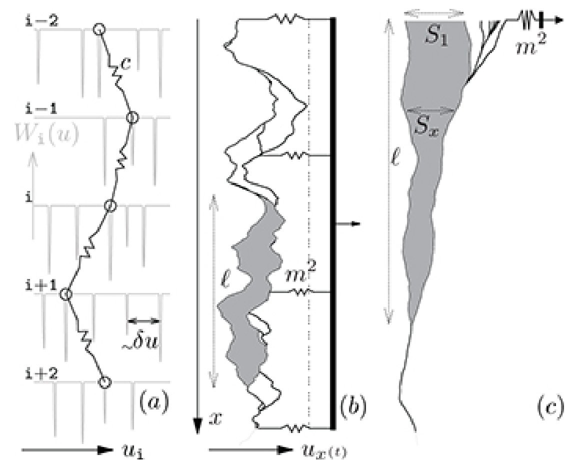
Driven interface over a disordered background



A line



Depinning & creep



avalanches

e.g. review **Giamarchi et al 05**, connections to earthquakes **Landes 16**

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Active matter

Definition

Active matter is composed of large numbers of active "agents", each of which consumes energy in order to move or to exert mechanical forces.

Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.

Energy injection is done “uniformly” within the samples (and not from the borders).

Coupling to the environment (bath) allows for the dissipation of the injected energy.

Active matter

Introduction

- Scales: macroscopic to microscopic

  Natural examples are birds, fish, cells, bacteria.

- Also artificial realisations: Janus particles, granular like, etc.

- $3d$, $2d$ and $1d$.

- Modelling: very detailed to coarse-grained or schematic.

  — microscopic or *ab initio* with focus on active mechanism,

  — *mesoscopic*, just forces that do not derive from a potential,

  — *Cellular automata* like in the Vicsek model.

Natural systems

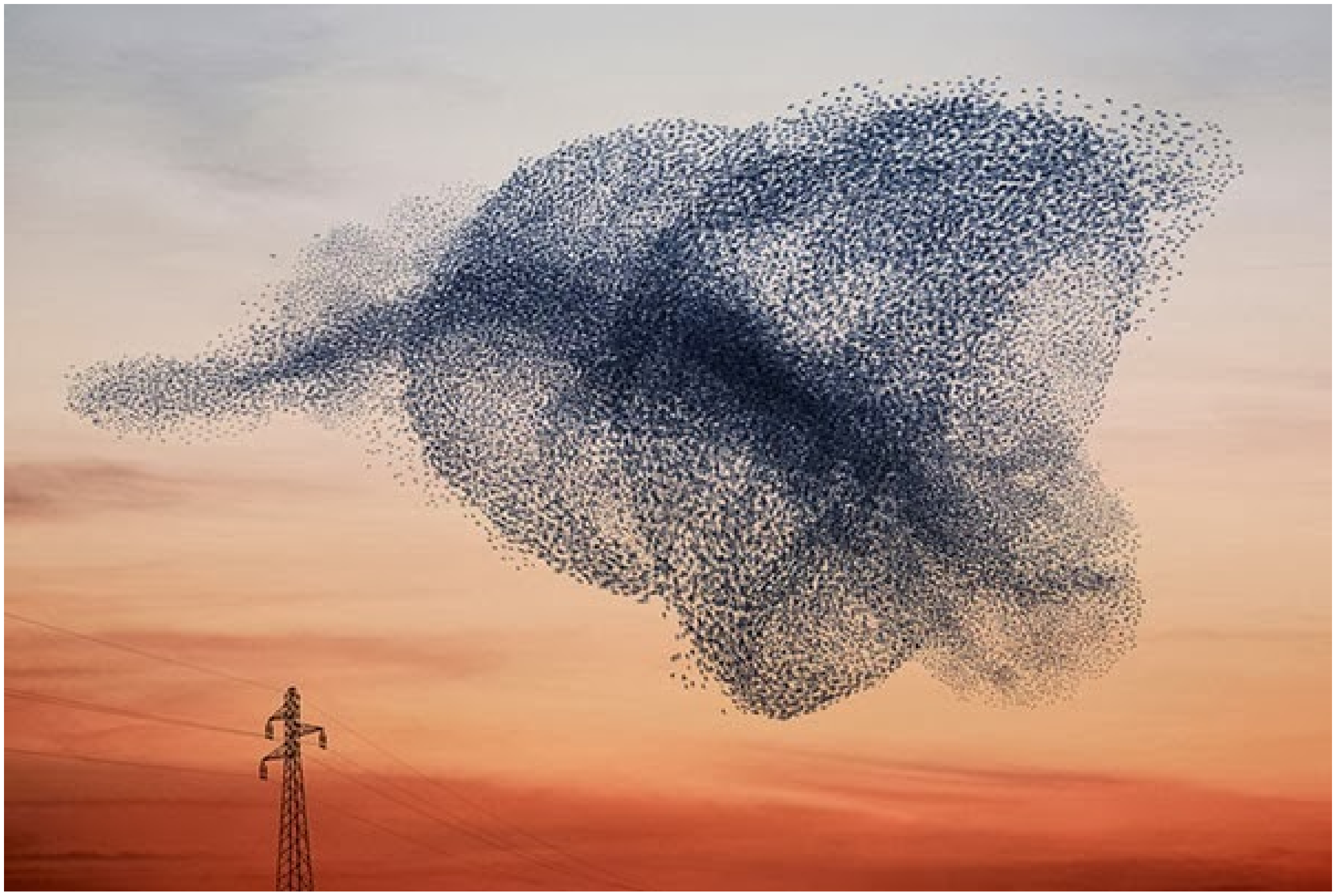
Birds flocking

Natural systems

Birds flocking

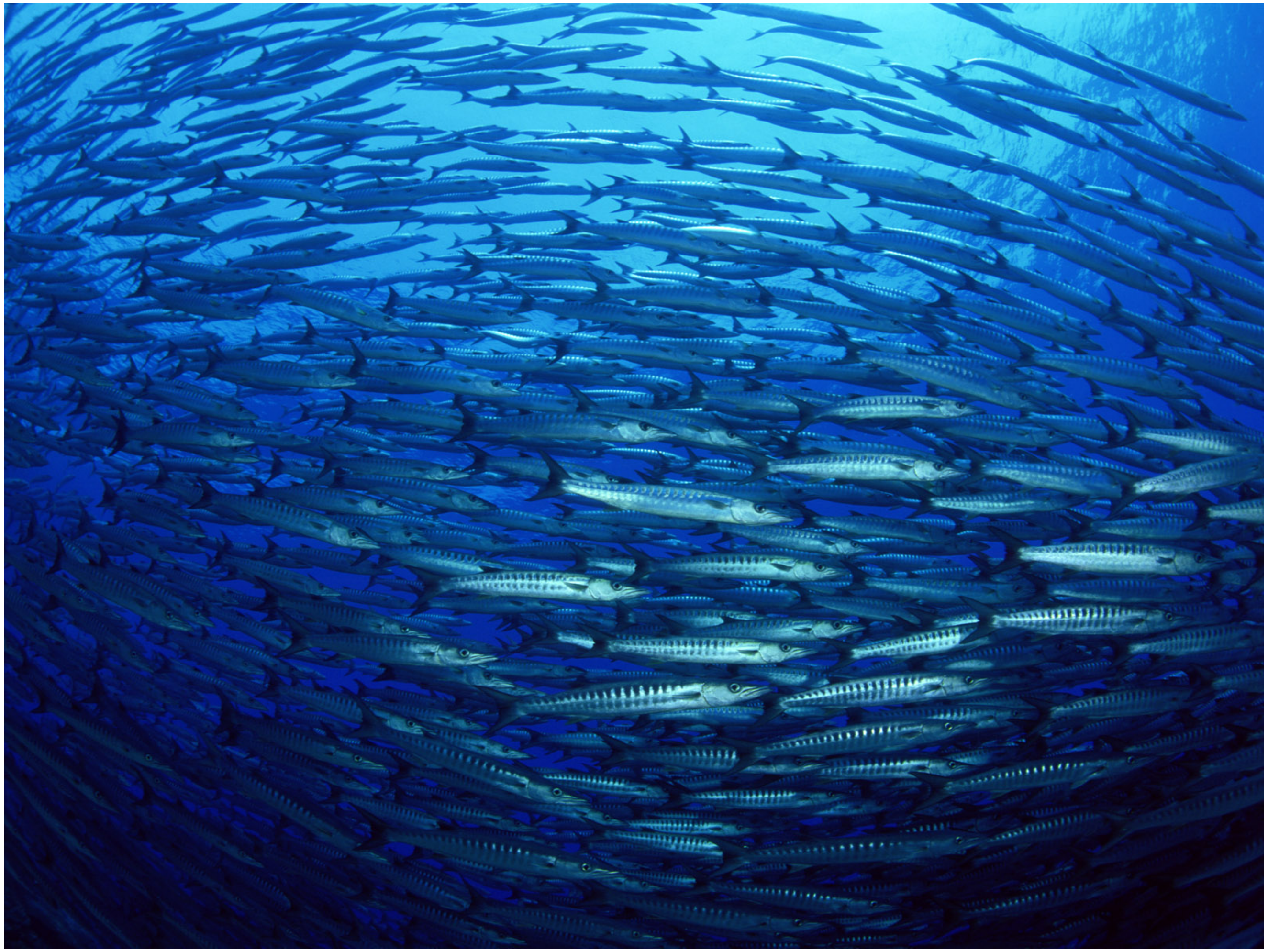
Natural systems

Birds flocking



Natural systems

School of fish



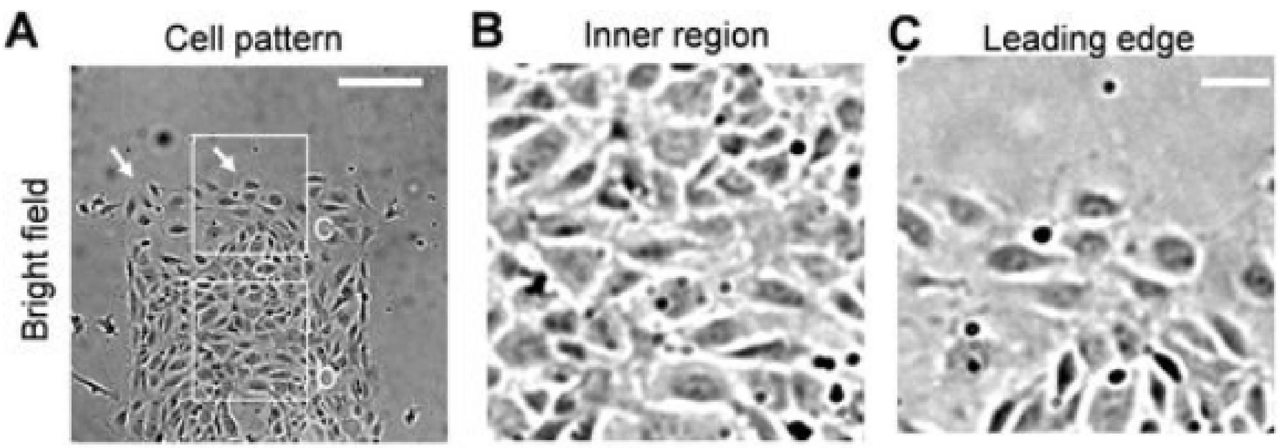
Natural systems

School of fish

Natural systems

Cell migration

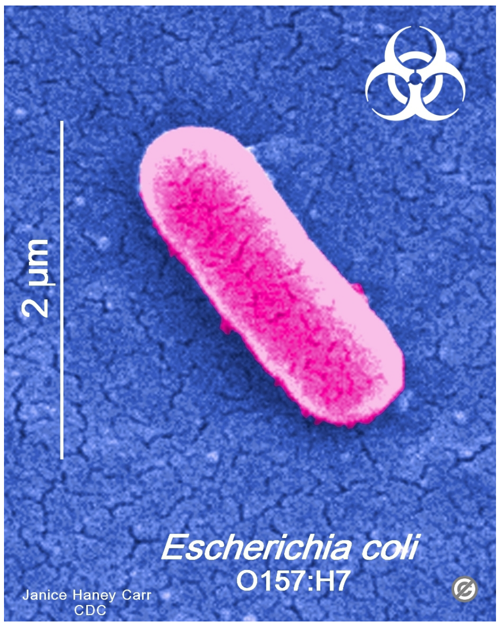
Collective cell migration is the process whereby a group of cells move in concert, without completely disrupting their cell-cell contacts. Collective migration is important during morphogenesis, and in pathological processes such as wound healing and cancer cell invasion.

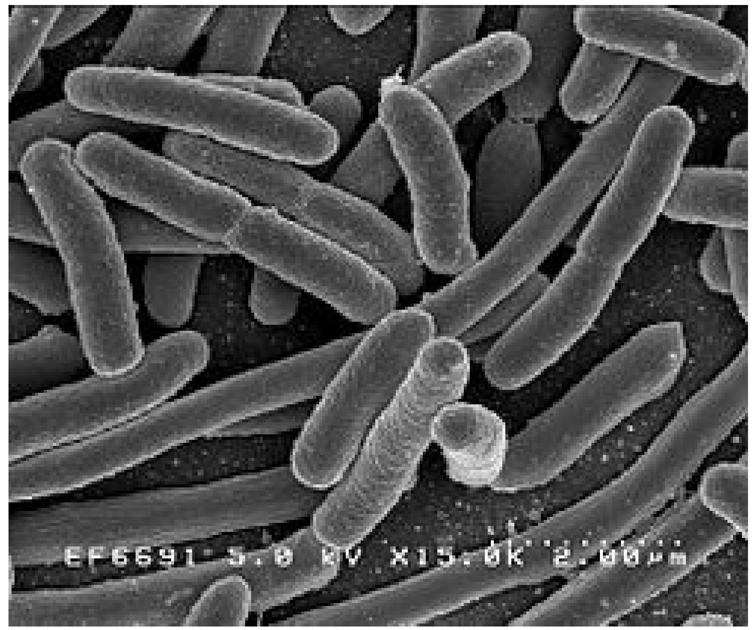


Physicists approach : **Jülicher, Joanny, Shraiman, etc.**

Natural systems

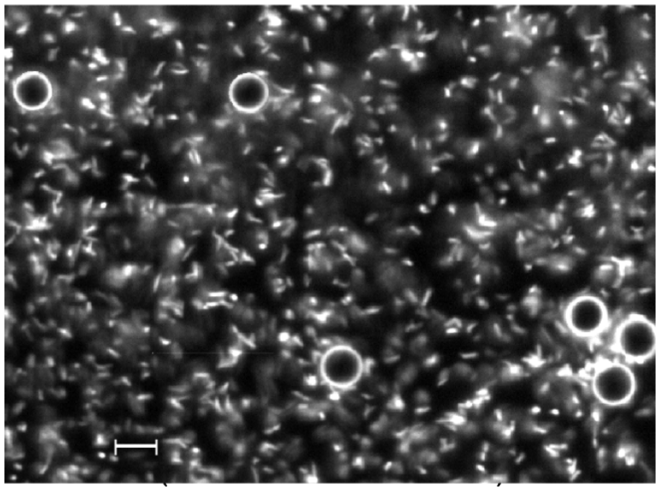
Bacteria





Escherichia coli - Pictures borrowed from the internet.

An active bath



(Influential paper)

Dynamics of an *open system*

The system : the Brownian particle

A double bath : bacteria suspension

Interaction

'Canonical setting'

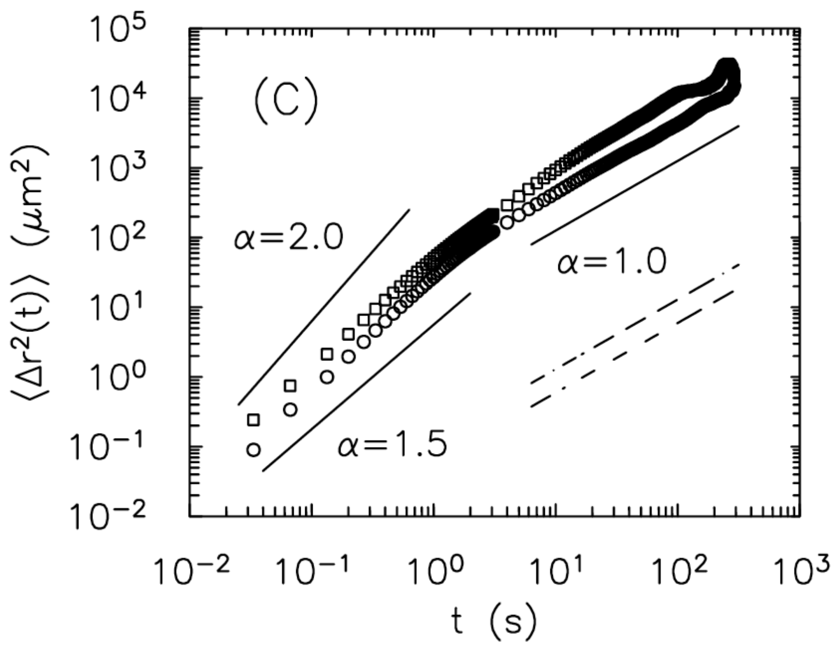
A few Brownian particles or tracers ● imbedded in an active bath

"Particle Diffusion in a Quasi-Two-Dimensional Bacterial Bath"

Wu & Libchaber, Phys. Rev. Lett. 84, 3017 (2000)

An active bath

Enhanced diffusion



Mean-square displacement of the Brownian particle

crossover form super-diffusion to diffusion

enhanced diffusion constant: effective temperature

(more later)

A few Brownian particles or tracers • imbedded in an active bath

"Particle Diffusion in a Quasi-Two-Dimensional Bacterial Bath"

Wu & Libchaber, Phys. Rev. Lett. 84, 3017 (2000)

Artificial systems

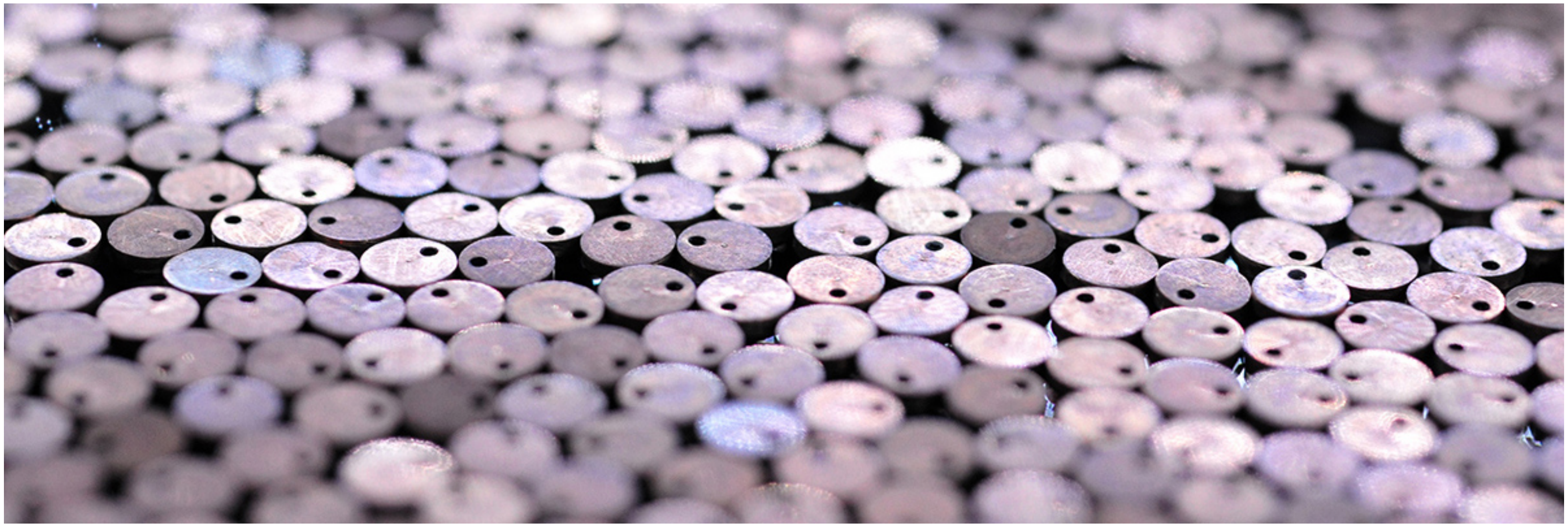
Nano HexBugs on a table

Propulsion: batteries

e.g., **Ciliberto group ENS-Lyon**

Artificial systems

Granular walkers on the plane



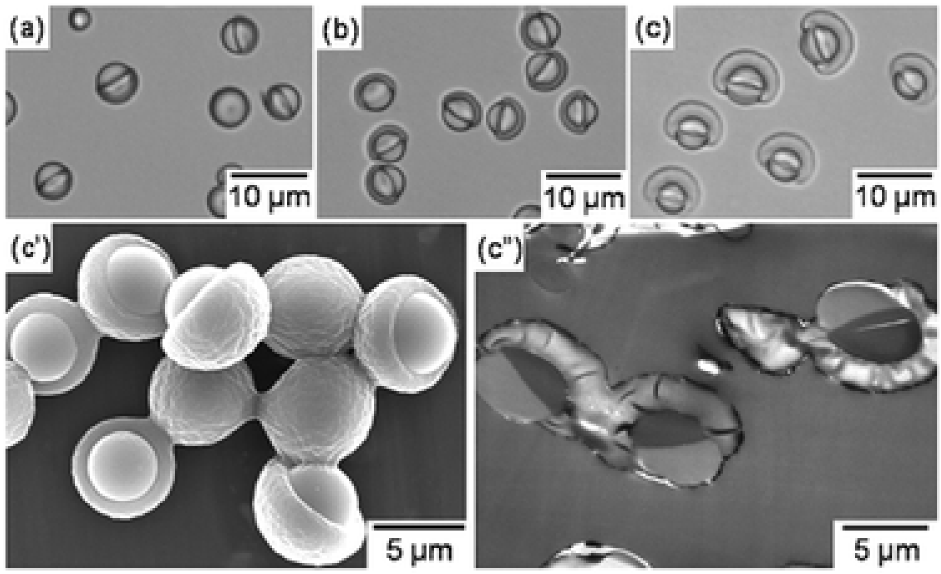
Asymmetric particles

Propulsion: baseline vibration of disordered plane

e.g., **Dauchot group** ESPCI-Paris, **Menon group** Amherst

Artificial systems

Janus particles



Particles with two faces (Janus God)

e.g. **Bocquet group** ENS Lyon-Paris, **di Leonardo group** Roma

Microscopic scales

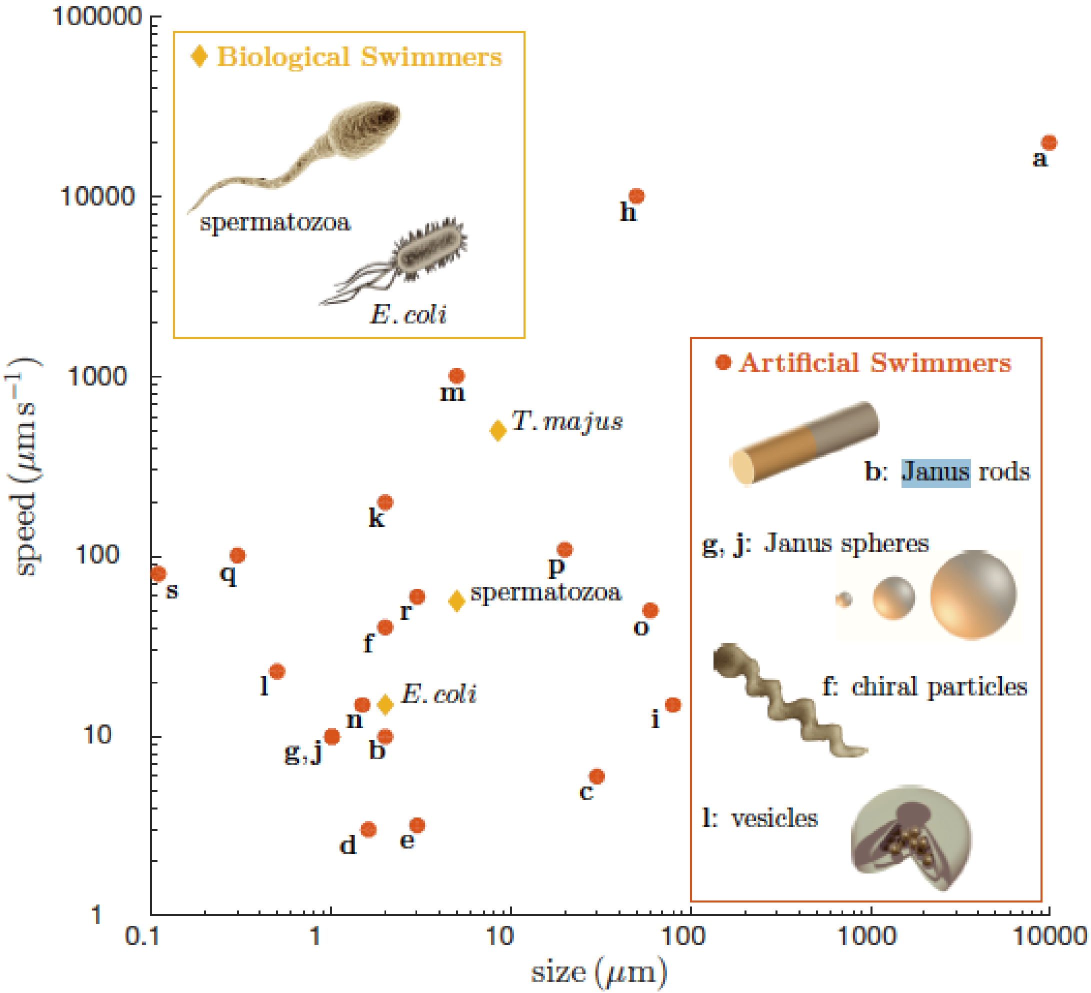


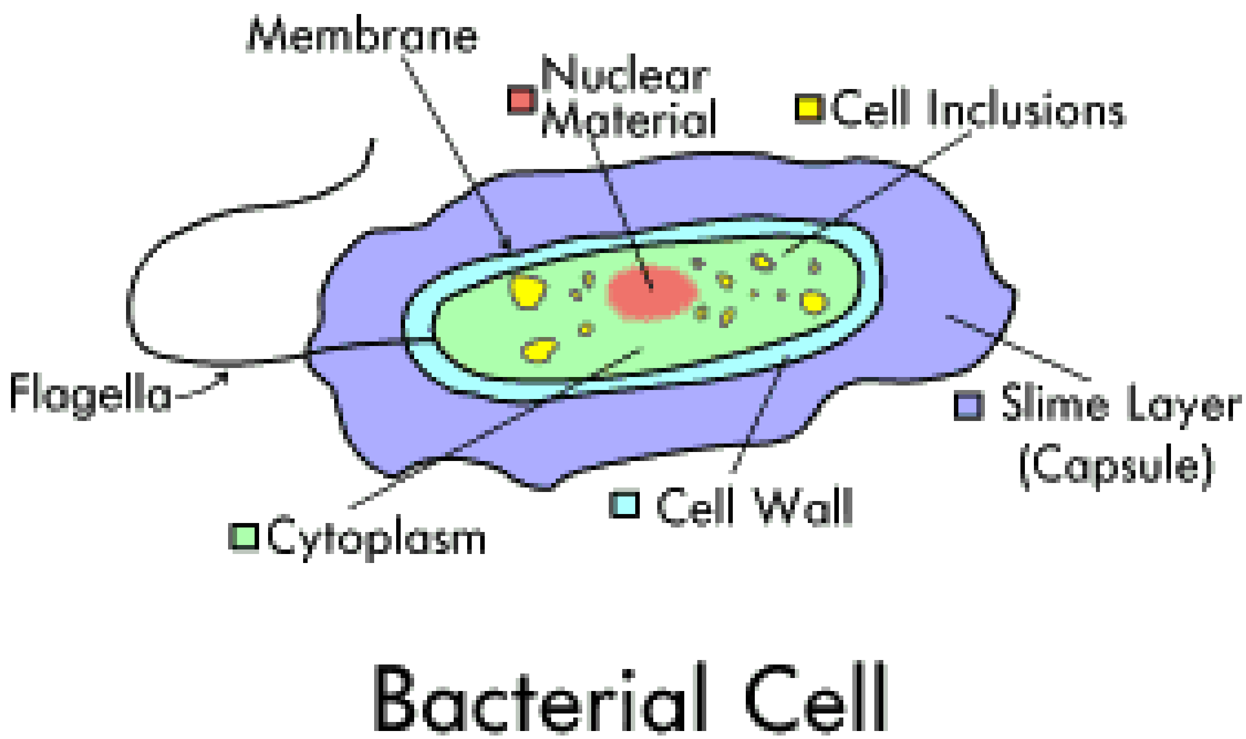
Image taken from **Bechinger et al, Rev. Mod. Phys. 88, 045006 (2016)**

Mechanisms of propulsion

Flying bird & swimming fish

Mechanisms of propulsion

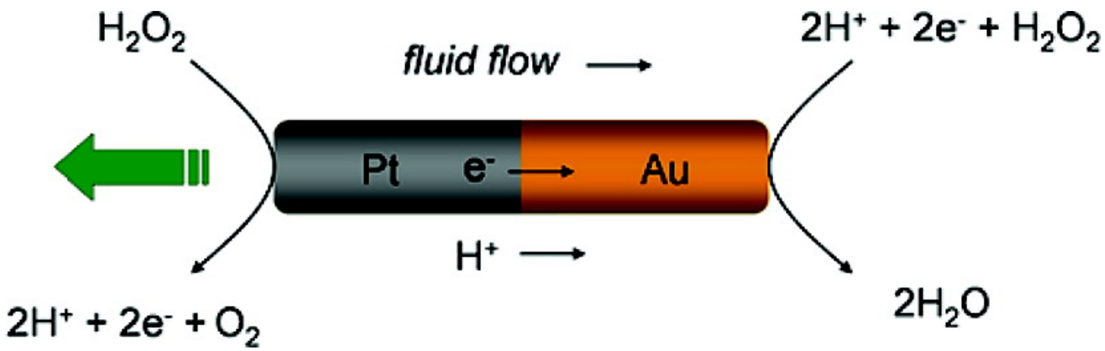
Bacteria



Flagella (whip), e.g. d = 20 nm, $\ell =$ 15-20 μm

Mechanisms of propulsion

Chemical



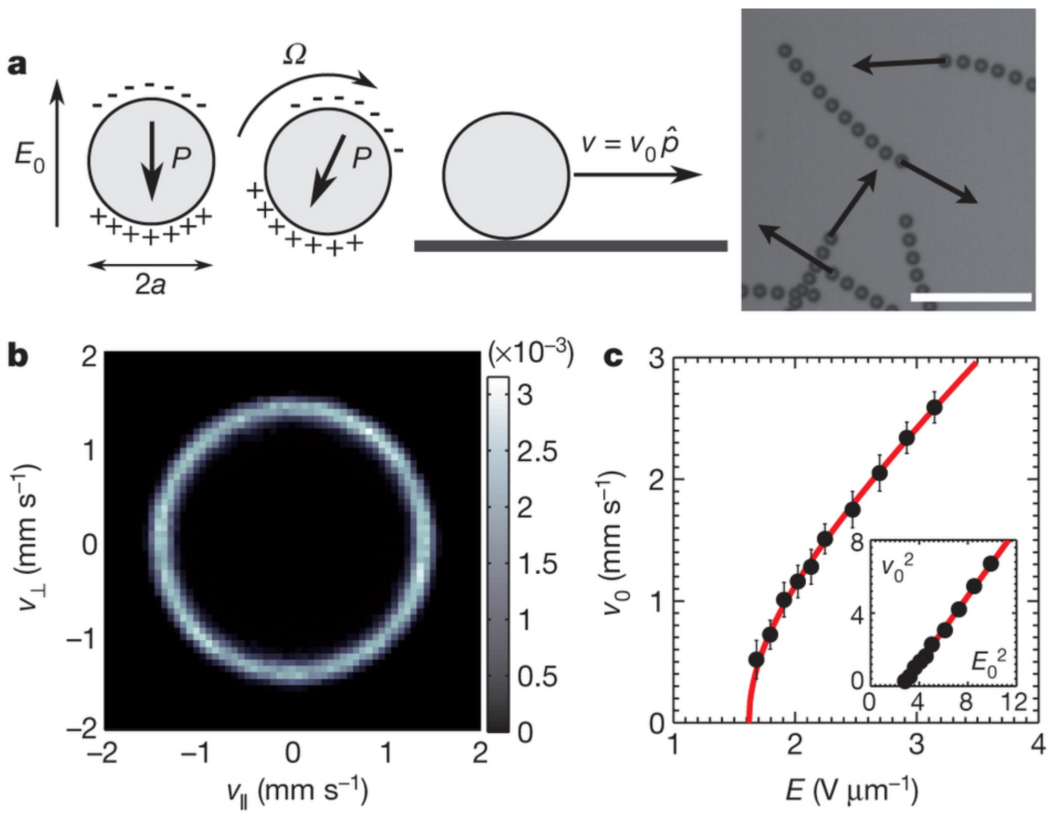
Self electrophoresis process

Paxton, Baker, Kline, Wang, Mallouk & Sen

Mitchell, *"Self-electrophoretic locomotion in microorganisms: bacterial flagella as giant ionophores"* **FEBS Lett. 28, 1 (1972)**

Mechanisms of propulsion

Colloidal rollers



"Emergence of macroscopic directed motion in populations of motile colloids"

Bricard, Caussin, Desreumaux, Dauchot & Bartolo, Nature 503, 95 (2013)

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Problem & questions

From single to many-body

- How does an atypical force, the active force, alter the dynamics of an object (with a given form and mass distribution) immersed in a thermal bath, i.e. subject to friction $\to$ dissipation and thermal fluctuations $\to$ noise.
- Collective effects of an ensemble of such objects in interaction.

  — Dynamic phase transitions ? $3d$ *vs.* $2d$?

  — Active solid, liquid, gas phases ?

  — Collective dynamics ?

Models & Methods

From very detailed to approximate

	Biological	Statistical physics	Non-linear dynamics
Microscopic		Brownian/Run&Tumble	Cellular automata
Collective		Phases & transitions	Bifurcations
Experiments		Soft-condensed matter	
Numerical		MD, MC, Lattice Boltzmann	Integration
Analytical		Liquid/Glass theory	Hydrodyn/Mechanics

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The position and velocity of an agent are $\boldsymbol{r}_i$ and $\boldsymbol{v}_i = v_0 \hat{\boldsymbol{v}}_i$ with $v_0 = \text{cst}$.

Each microscopic update is such that the individual's direction is updated according to the mean $\overline{\dots}$ over its neighbours

$$\hat{\boldsymbol{v}}_i(t+\delta t) = \overline{\hat{\boldsymbol{v}}_j(t)}_{|\boldsymbol{r}_i - \boldsymbol{r}_j| < r} + \boldsymbol{\eta}_i(t)$$

plus some noise $\boldsymbol{\eta}_i$ (normalisation is imposed after each step) and moves at constant speed v_0 in the new direction

$$\boldsymbol{r}_i(t+\delta t) = \boldsymbol{r}_i(t) + v_0 \hat{\boldsymbol{v}}_i(t+\delta t)\, \delta t$$

"Novel Type of Phase Transition in a System of Self-Driven Particles",

Vicsek, Czirók, Ben-Jacob, Cohen, Shochet, Phys. Rev. Lett. 75 1226 (1995)

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The particles are self-propelled due to v_0

The total number of particles is conserved (no birth/death).

The velocity direction plays a similar role to the one of the spin in the Heisenberg (or XY) ferromagnetic models (more later)

As the particles move in the direction of their velocity, the “connectivity matrix” is not constant, but evolves (if the interaction range is finite).

There is no momentum conservation and Galilean invariance is broken.

Spontaneous symmetry breaking of polar order, $\boldsymbol{p}(t) = \frac{1}{N} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t) \neq 0$

At $v_0 = 0$ the model is the Heisenberg one. However, this is a singular limit.

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The global behaviour is controlled by the density ϕ, the noise amplitude $k_B T$ and the particles' modulus of the velocity v_0.

Dynamic phase diagram $(k_B T, \phi)$ (v_0 fixed) from

the polar order parameter $\boldsymbol{p}(t) = \frac{1}{N} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t)$

- Homogenous collective motion (high density, weak noise)
- Ordered bands (intermediate)
- Disordered (low density, strong noise)

"Novel Type of Phase Transition in a System of Self-Driven Particles",

Vicsek, Czirók, Ben-Jacob, Cohen, Shochet, Phys. Rev. Lett. 75 1226 (1995)

Ginelli, arXiv:1511.01451 in Microswimmers Summer School, Jülich

Models

Continuum model

The mean center-of-mass velocity $\langle \boldsymbol{v} \rangle$ is the order parameter.

The development of $\langle \boldsymbol{v} \rangle \neq \mathbf{0}$ for the flock as a whole requires spontaneous breaking of the continuous rotational symmetry.

Out of equilibrium feature possible also in low dimensions.

Breakdown of linearized hydrodynamics imply large fluctuations in dimensions smaller than four.

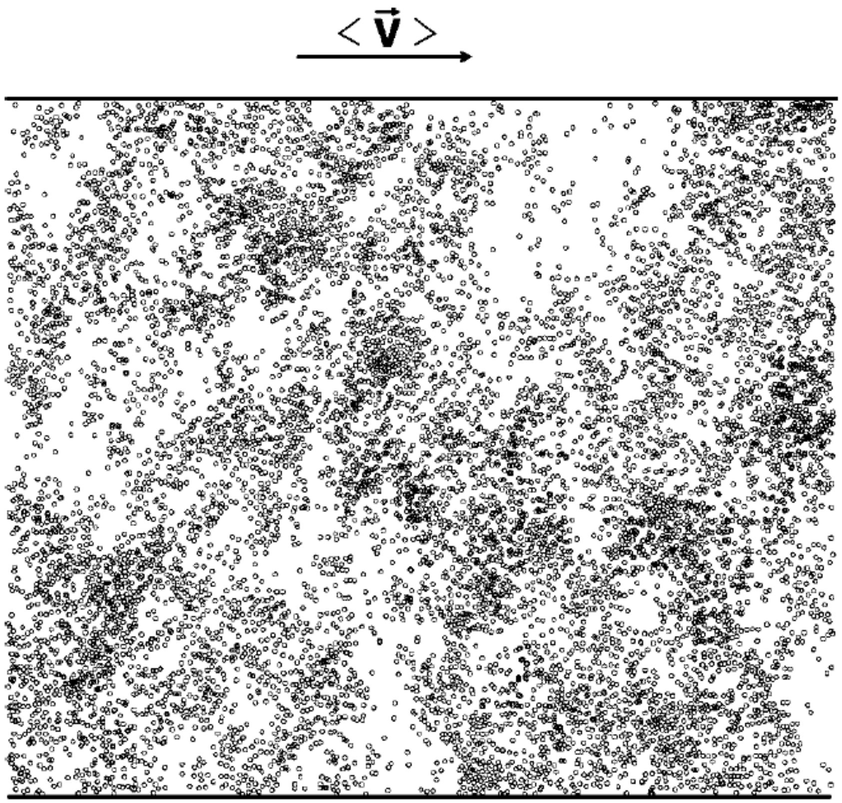
Argument: Improved transport suppresses the very fluctuations that give rise to it, leading to long-range order in $d = 2$.

"Flocks, herds, and schools : A quantitative theory of flocking",

Toner & Tu, Phys. Rev. E 58, 4828 (1998)

Models

Continuum model : giant density fluctuations



"Long-Range Order in a $2d$ Dynamical XY Model : How Birds Fly Together"

"Flocks, herds, and schools : A quantitative theory of flocking",

J. Toner & Y. Tu, Phys. Rev. Lett. 75, 4326 (1995), Phys. Rev. E 58, 4828 (1998)

Models

Continuum model

$$\partial_t \boldsymbol{v} + \underbrace{\lambda_1 (\boldsymbol{\nabla} \cdot \boldsymbol{v})\boldsymbol{v} + \lambda_2 (\boldsymbol{v} \cdot \boldsymbol{\nabla})\boldsymbol{v} + \lambda_3 \boldsymbol{\nabla} v^2}_{\text{Navier-Stokes w/no Galilean invariance}} =$$

$$\underbrace{\alpha_1 \boldsymbol{v} - \alpha_2 v^2 \boldsymbol{v}}_{\text{“Potential force” imposing } v^2 = \alpha_1/\alpha_2} \qquad \underbrace{-\boldsymbol{\nabla} P}_{\text{“Pressure variation”}}$$

$$\underbrace{+ D_B \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{v}) + D_T \nabla^2 \boldsymbol{v} + D_2 (\boldsymbol{v} \cdot \boldsymbol{\nabla})^2 \boldsymbol{v}}_{\text{Dissipative terms}} \underbrace{+ \boldsymbol{\eta}}_{\text{Noise}}$$

$$P = \sum_{n=1}^{\infty} \sigma_n (\rho - \rho_0)^n$$

Pressure tending to impose $\rho - \rho_0$ small

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\boldsymbol{v}\rho) = 0$$

Toner & Tu, Phys. Rev. E 58, 4828 (1998)

$\alpha_1 < 0$ ($\alpha_1 > 0$) in the homogenous (flocking) phase

“Hydrodynamic eqs. for self-propelled part.: microscopic derivation & stability analysis”

Bertin, Droz and Grégoire, J. Phys. A 42, 445001 (2009)

Models

Run & tumble particles

This mechanism can be described as a repeating sequence of two actions:

(i) a period of nearly constant-velocity translation (run) followed by

(ii) a seemingly erratic rotation (tumble).

Observed by **Berg & Brown, Nature (1972)**

Simulation from **M. Kardar**'s webpage

Run with $v = 20\,\mu m/s$; tumble with rate $\alpha = 1/s$ and duration $\tau = 0.1\,s$

Diffusion constants

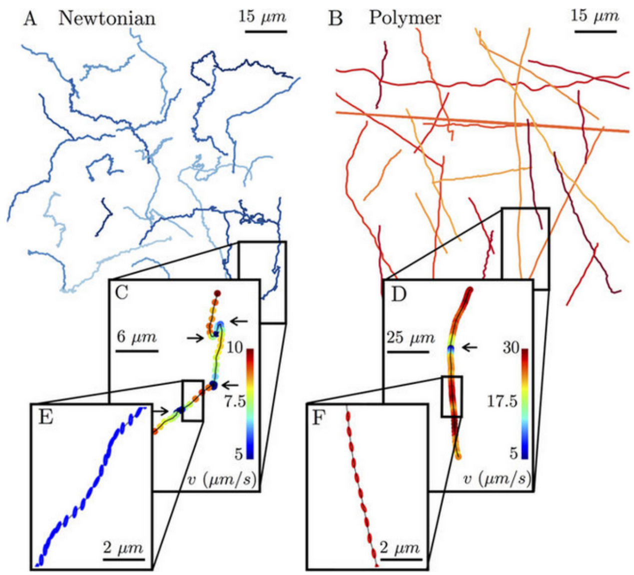
$$D_{RT} = \frac{v^2}{d\alpha(1+\alpha\tau)} \simeq 100\,\mu m^2/s$$

$$D_{BM} = \frac{k_B T}{6\pi\eta R} \simeq 0.2\,\mu m^2/s$$

Models

Run & tumble particles

Some trajectories depending on the environment



Trajectories of E. coli cells in (A) buffer and (B) polymeric solution

"Running and tumbling with E. coli in polymeric solutions",

Patteson, Gopinath, Goulian and Arratia, Scient. Rep. 5, 15761 (2015)

Models

Fluctuating hydrodynamic theories in low density limits

Local density scalar field $\rho(\boldsymbol{r},t) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$

Local polar vector field $\boldsymbol{p}(\boldsymbol{r},t) = \frac{1}{\rho(\boldsymbol{r},t)} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t)\delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$

$$
\begin{aligned}
\partial_t \rho + v_0 \boldsymbol{\nabla} \cdot (\rho \boldsymbol{p}) &= -\boldsymbol{\nabla} \cdot \left(-\frac{1}{\gamma_\rho} \boldsymbol{\nabla} \frac{\delta F}{\delta \rho} + \boldsymbol{\eta}_\rho \right) \\
\partial_t \boldsymbol{p} + \lambda_1 (\boldsymbol{p} \cdot \boldsymbol{\nabla}) \boldsymbol{p} &= -\frac{1}{\gamma_{\boldsymbol{p}}} \frac{\delta F}{\delta \boldsymbol{p}} + \boldsymbol{\eta}_{\boldsymbol{p}}
\end{aligned}
$$

with wise proposals for the “free-energy” F and noises $\boldsymbol{\eta}_\rho$ and $\boldsymbol{\eta}_{\boldsymbol{p}}$.

“Hydrodynamics of soft active matter”

Marchetti, Joanny, Ramaswamy, Liverpool, Prost, Rao, Simha

Rev. Mod. Phys. 85 (2013)

Models

Focus on simpler ones

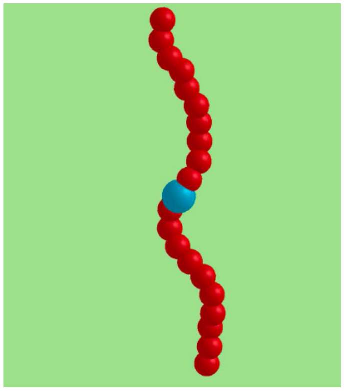
Homogenous energy injection, contrary to rheology (from boundaries)

Non-persistent

Change in time, in direction, where they

are applied,

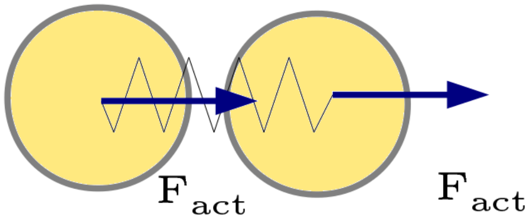
on point-like or elongated particles



Persistent

Constant strength,

axial direction



Problem & questions

From single to many-body

- How does an atypical force, the active force, alter the dynamics of an object (with a given form and mass distribution) immersed in a thermal bath, i.e. subject to friction $\longrightarrow$ dissipation and thermal fluctuations $\longrightarrow$ noise.

- Collective effects of an ensemble of such objects in interaction.

  — Translational and rotational motion.

  — Fluctuation-dissipation theorem & effective temperatures.

  — Phases.

Plan

5 lectures & 2 exercise sessions

1. **Introduction**
2. Active Brownian dumbbells
3. Effective temperatures
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

Some reviews: **Vicsek 10, Fletcher & Geissler 09, Menon 10, Ramaswamy 10, Romanczuk et al 12, Cates 12, Marchetti et al. 13, de Magistris & Marenduzzo 15**