Active Matter

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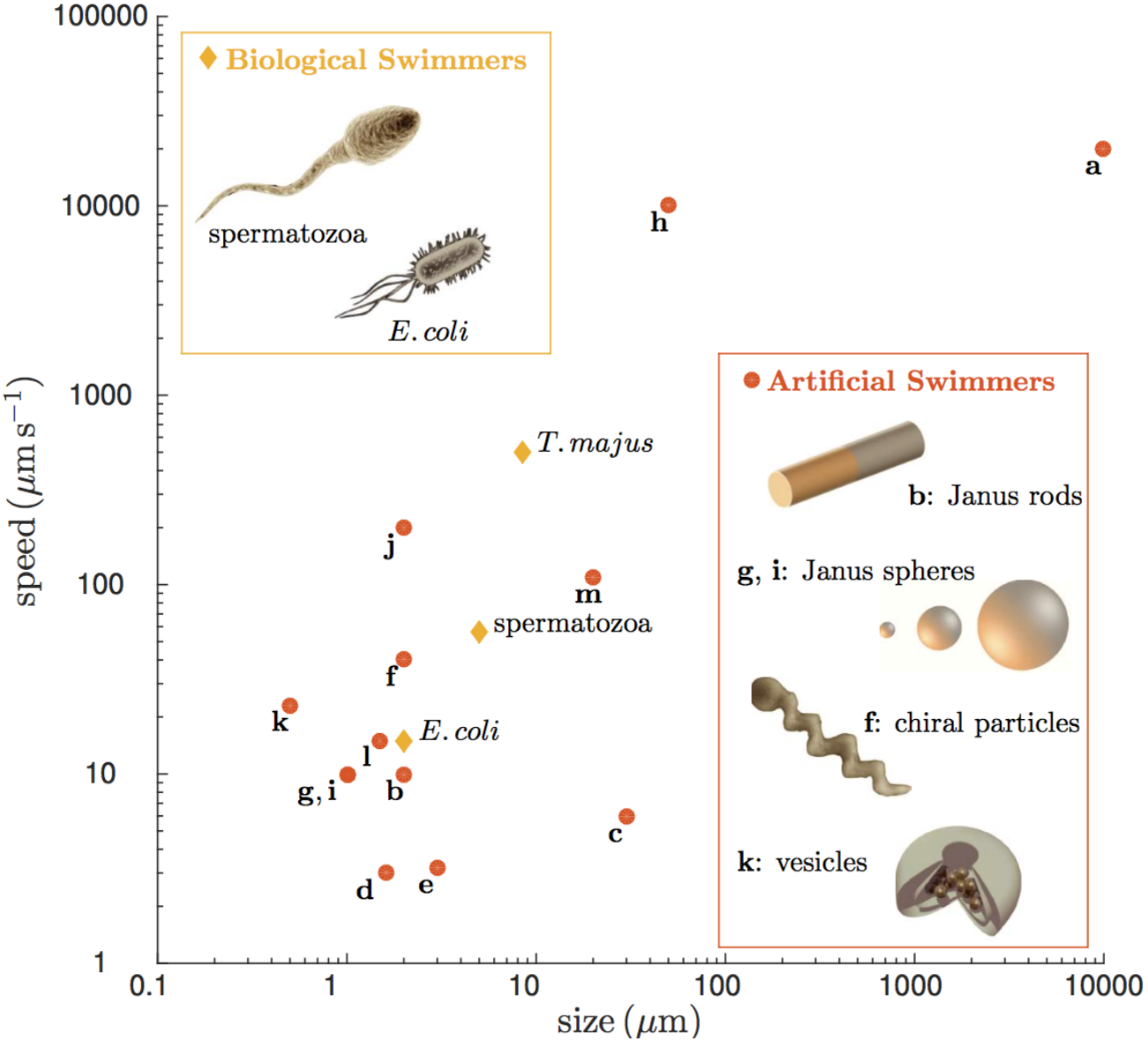
September 6, 2016

Active matter: Biological, but also synthetic systems

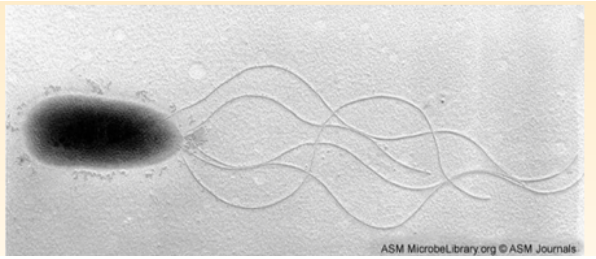


	Microswimmer	Propulsion mechanism	Medium	Dimensions	Max. Speed
a	PDMS platelets coated with Pt (Ismagilov *et al.*, 2002)	Bubbles generated in a H_2O_2 aqueous solution by asymmetric patterns of Pt	H_2O_2 aqueous meniscus	1 cm	$2\,\mathrm{cm\,s^{-1}}$
b	Rod-shaped particles consisting of Au and Pt segments (Paxton *et al.*, 2004)	Catalysis of oxygen at the Pt end of the rod	Near a boundary in H_2O_2 acqueous solution	$2\,\mu$m (length), 370 nm (width)	$10\,\mu\mathrm{m\,s^{-1}}$
c	Linear chains of DNA-linked magnetic colloidal particles attached to red blood cells (Dreyfus *et al.*, 2005)	External actuation of the flexible artificial flagella by oscillating magnetic fields	Aqueous solution	$30\,\mu$m	$6\,\mu\mathrm{m\,s^{-1}}$
d	Janus spherical particles with a catalytic Pt patch (Howse *et al.*, 2007)	Self-diffusiophoresis catalyzed by a chemical reaction on the Pt surface	H_2O_2 aqueous solution	$1.6\,\mu$m	$3\,\mu\mathrm{m\,s^{-1}}$
e	DNA-linked anisotropic doublets composed of paramagnetic colloidal particles (Tierno *et al.*, 2008)	Rotation induced by a rotating magnetic field	Near a boundary in aqueous solution	$3\,\mu$m	$3.2\,\mu\mathrm{m\,s^{-1}}$
f	Chiral colloidal propellers (Ghosh and Fischer, 2009)	External actuation by a magnetic field	Aqueous solution	$2\,\mu$m (length), 250 nm (width)	$40\,\mu\mathrm{m\,s^{-1}}$
g	Janus particles half-coated with Au (Jiang *et al.*, 2010)	Self-thermophoresis due to local heating at the Au cap	Aqueous solution	$1\,\mu$m	$10\,\mu\mathrm{m\,s^{-1}}$
h	Catalytic microjets (Sanchez *et al.*, 2011)	H_2O_2 catalysis on the internal surface of the microjet	H_2O_2 aqueous solution	$50\,\mu$m (length), $1\,\mu$m (width)	$10\,\mathrm{mm\,s^{-1}}$
i	Janus particles with light-absorbing patches (Buttinoni *et al.*, 2012; Kümmel *et al.*, 2013; Volpe *et al.*, 2011)	Local demixing of a critical mixture due to heating associated to localized absorption of light	Critical mixture (e.g. water-2,6-lutidine)	0.1 to $10\,\mu$m	$10\,\mu\mathrm{m\,s^{-1}}$
j	Rod-shaped particles consisting of Au and Pt (or Au and Ru) segments (Wang *et al.*, 2012)	Self-acoustophoresis in a ultrasonic standing wave	Aqueous solution	1 to $3\,\mu$m (length), 300 nm (width)	$200\,\mu\mathrm{m\,s^{-1}}$
k	Pt-loaded stomatocytes (Wilson *et al.*, 2012)	Bubbles generated in a H_2O_2 aqueous solution by entrapped Pt nanoparticles.	H_2O_2 acqueous solution	$0.5\,\mu$m	$23\,\mu\mathrm{m\,s^{-1}}$
l	Polymeric spheres encapsulating most of an antiferromagnetic hematite cube (Palacci *et al.*, 2013)	Self-phoretic motion near a boundary due to the decomposition of H_2O_2 by the hematite cube when illuminated by ultraviolet light	Near a boundary in H_2O_2 acqueous solution	$1.5\,\mu$m	$15\,\mu\mathrm{m\,s^{-1}}$
m	Janus microspheres with Mg core, Au nanoparticles, and TiO_2 shell layer (Li *et al.*, 2014)	Bubble thrust generated from the Mg-water reaction	Aqueous solution	$20\,\mu$m	$110\,\mu\mathrm{m\,s^{-1}}$

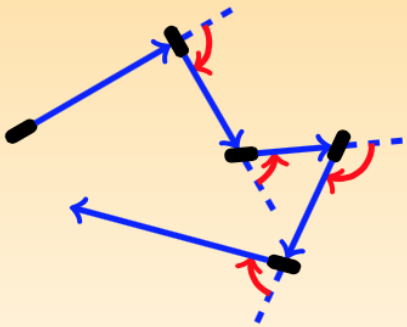
Active matter

- A large numbers of active "agents", each of which consumes energy in order to move.
- Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.
- Every particle in an active matter system is out of equilibrium, in contrast to 'boundary driven' systems, like a strip of metal heated at one end, that are locally equilibrated.
- Schools of fish, flocks of birds, bacteria, artificial self-propelled particles, and self-organising bio-polymers such as microtubules and actin.
- Analytical approaches include hydrodynamics, kinetic theory, and non-equilibrium statistical physics. Numerical studies mainly involve self-propelled-particles models, making use of agent-based techniques and molecular dynamics algorithms.

Self Propulsion in Berg's Run and tumble non-interacting model



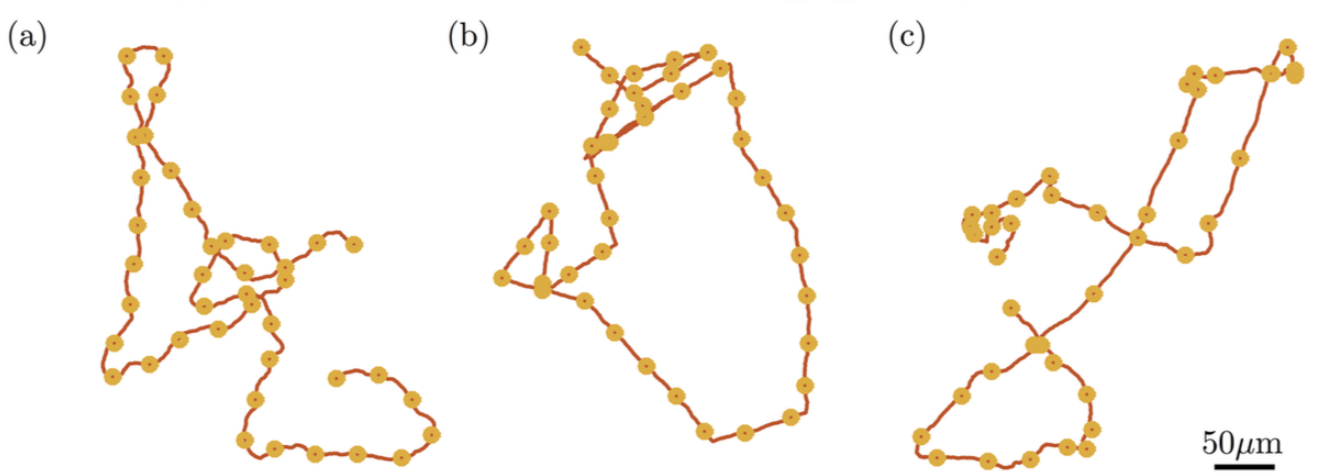
- Run: straight line (velocity $v \simeq 20\,\mu\mathrm{m.s}^{-1}$) •
- Tumble: change of direction (rate $\alpha \simeq 1\,\mathrm{s}^{-1}$, duration $\tau \simeq 0.1s$) •



- Diffusion at large scale
  - Run-and-Tumble $D = \frac{v^2}{d\alpha(1+\alpha\tau)} \sim 100\,\mu m^2.s^{-1}$
  - Brownian Motion $D_{col} = \frac{kT}{6\pi\eta r} \sim 0.2\mu m^2.s^{-1}$

Run and Tumble and Active Brownian particles models

Cells alternate periods of smooth forward swimming (runs) with abrupt reorientations (tumbles).



Active Brownian

$$\dot{\mathbf{x}}_i(t) = v_0 \mathbf{e}_i(t) + \frac{\mathbf{F}_i}{\gamma} \quad , \qquad \dot{\theta}_i(t) = \sqrt{D_r}\eta_i^{\theta}(t), \quad D = \frac{v_0^2}{2D_r}$$

Gaussian colored noise model

$$\dot{\mathbf{x}}_i(t) = \mathbf{u}_i(t) + \frac{\mathbf{F}_i}{\gamma} \quad , \qquad \dot{\mathbf{u}}_i(t) = -\frac{1}{\tau}\mathbf{u}_i(t) + \frac{D^{1/2}}{\tau}\eta_i(t)$$

Interacting active systems

Overdamped dynamics of N of degrees of freedom $(x_1, \ldots, x_N)$:

$$\frac{dx_i}{dt} = -\frac{\partial U}{\partial x_i} + \eta_i(t) \tag{1}$$

$U(x_1, \ldots, x_N)$ is a potential energy and $\eta_i(t)$ is an exponentially correlated colored noise satisfying

$$\langle \eta_i(t) \rangle = 0, \qquad \langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij} \frac{D}{\tau} e^{-|t-t'|/\tau} \,. \tag{2}$$

The exponentially correlated colored noise $\eta_i(t)$ can be interpreted as resulting from an Ornstein-Uhlenbeck process,

$$\frac{d\eta_i}{dt} = -\frac{\eta_i}{\tau} + \frac{1}{\tau}\xi_i(t) \tag{3}$$

where $\xi_i(t)$ is a white noise satisfying

$$\langle \xi_i(t) \rangle = 0, \qquad \langle \xi_i(t)\xi_j(t') \rangle = 2T\delta_{ij}\delta(t-t') \tag{4}$$

$$T = D\gamma$$

Taking the time derivative of Eq. (1) and combining the resulting equation with Eq. (3), one obtains

$$\tau\frac{d^2x_i}{dt^2} + \sum_j \left(\delta_{ij} + \tau\frac{\partial^2 U}{\partial x_i \partial x_j}\right)\frac{dx_i}{dt} = -\frac{\partial U}{\partial x_i} + \xi_i(t). \tag{5}$$

The Unified Colored Noise Approximation consists in neglecting the second derivative term in Eq. (5) The approximation is assumed to be valid both for $\tau \to 0$ and for $\tau \to \infty$

Unified color approximation equation

Dropping the second order time derivative (analogous to Kramers $\rightarrow$ Smoluchowski reduction)

$$\frac{dx_i}{dt} = -\sum_j (M^{-1})_{ij} \frac{\partial U}{\partial x_j} + \sum_j (M^{-1})_{ij} \xi_j(t) \tag{6}$$

which is a multiplicative Langevin equation, to be interpreted in the Stratonovich sense.

$$M_{ij} = \delta_{ij} + \tau \frac{\partial^2 U}{\partial x_i \partial x_j} \,. \tag{7}$$

Distribution of positions of N interacting persistent random walkers

For the N interacting particles, the probability distribution $P(x_1, \ldots, x_N, t)$ is ruled by the following Fokker-Planck equation,

$$\frac{\partial P}{\partial t} = \sum_i \frac{\partial J_i}{\partial x_i} \tag{8}$$

where the probability current $J_i(x_1, \ldots, x_N, t)$ is given by

$$J_i = \sum_j (M^{-1})_{ij} \frac{\partial U}{\partial x_j} P + T \sum_{j,k} (M^{-1})_{ij} \frac{\partial}{\partial x_k} [(M^{-1})_{jk} P] \,. \tag{9}$$

Consider the stationary solution of Eq. (8) with vanishing current, $J_i = 0$. Jacobi's formula

$$\frac{\partial}{\partial x_i} \ln |\det M| = \mathrm{Tr} \left(M^{-1} \frac{\partial M}{\partial x_i} \right), \tag{10}$$

The condition of vanishing probability current $J_i = 0$ leads to

$$\frac{\partial P}{\partial x_i} = \left(-\frac{1}{T} \sum_j M_{ij} \frac{\partial U}{\partial x_j} + \frac{\partial}{\partial x_i} \ln |\det M| \right) P \,. \tag{11}$$

Recalling the definition (7) of the matrix M, the stationary distribution $P(x_1, \ldots, x_N)$ is obtained as

$$P = \frac{1}{Z} |\det M| \exp \left[-\frac{U}{T} - \frac{\tau}{2T} \sum_i \left(\frac{\partial U}{\partial x_i} \right)^2 \right] \tag{12}$$

with Z a normalization constant. Eq. (12) generalizes the Boltzmann-Gibbs probability distribution, and reduces to it in the limiting case $\tau = 0$.

Detailed balance is satisfied by UCNA...

Notice Many body nature of the effective potential, even when U is a sum of pairwise potentials.

Consequence: Attraction out of repulsion.

The conditional distribution of velocity at fixed positions $\Pi(\mathbf{v}|\mathbf{x})$

At order τ is a Gaussian distribution

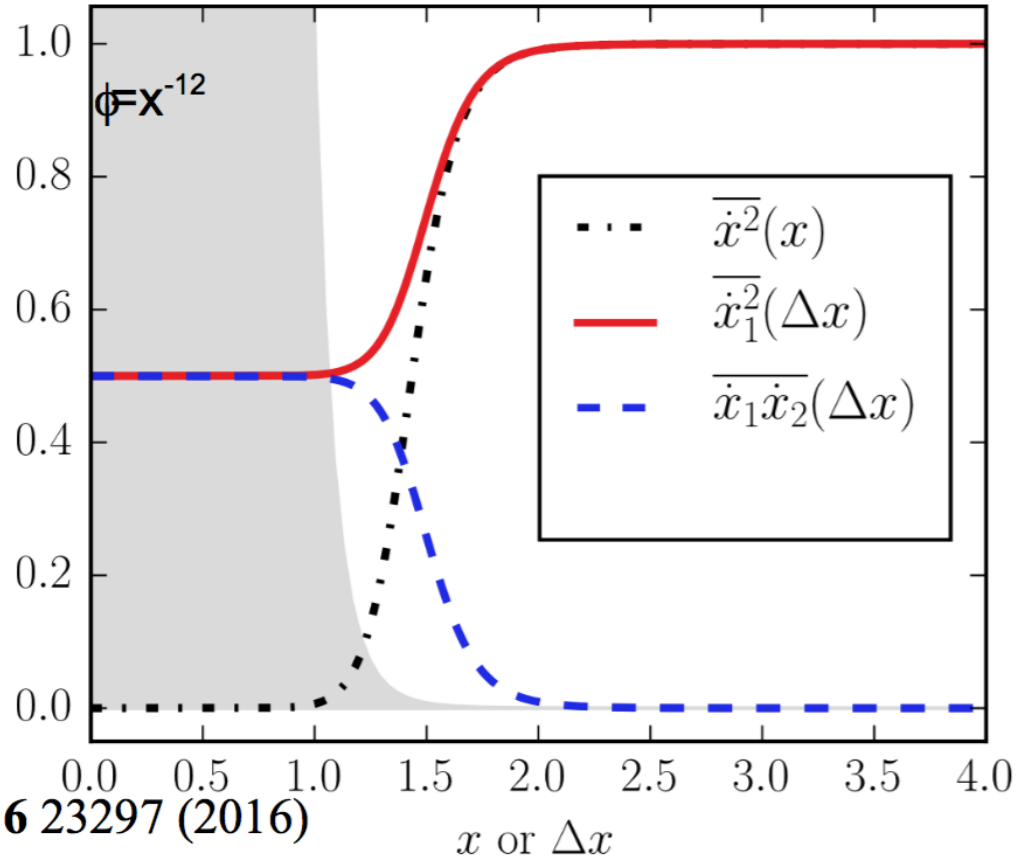
$$\Pi((\{v_i\}|\{x_i\}) = (\frac{\tau}{2\pi D})^{N/2}\sqrt{\det M}\,\exp\Big(-\frac{\tau}{2D_a}\sum_{ij} v_i M_{ij}(\{x\})v_j\Big) \quad (13)$$

Using the Gaussianity of the distribution we can immediately write the averages of the velocity as

$$< v_i v_j >= \int d^N x\, \overline{v_i v_j} P_N(\{x_i\}) = \frac{D_a}{\tau}\int d^N x M_{ij}^{-1}(\{x_i\})P_N(\{x_i\}) \quad (14)$$

Two nearby particles have correlated velocities

$$\overline{\dot{x}_1\dot{x}_2}(\Delta x) = \int d\dot{x}_1 d\dot{x}_2\, \dot{x}_1\dot{x}_2\, \Pi = \frac{D}{\tau}\frac{\tau\phi''(\Delta x)}{1+2\tau\phi''(\Delta x)}$$



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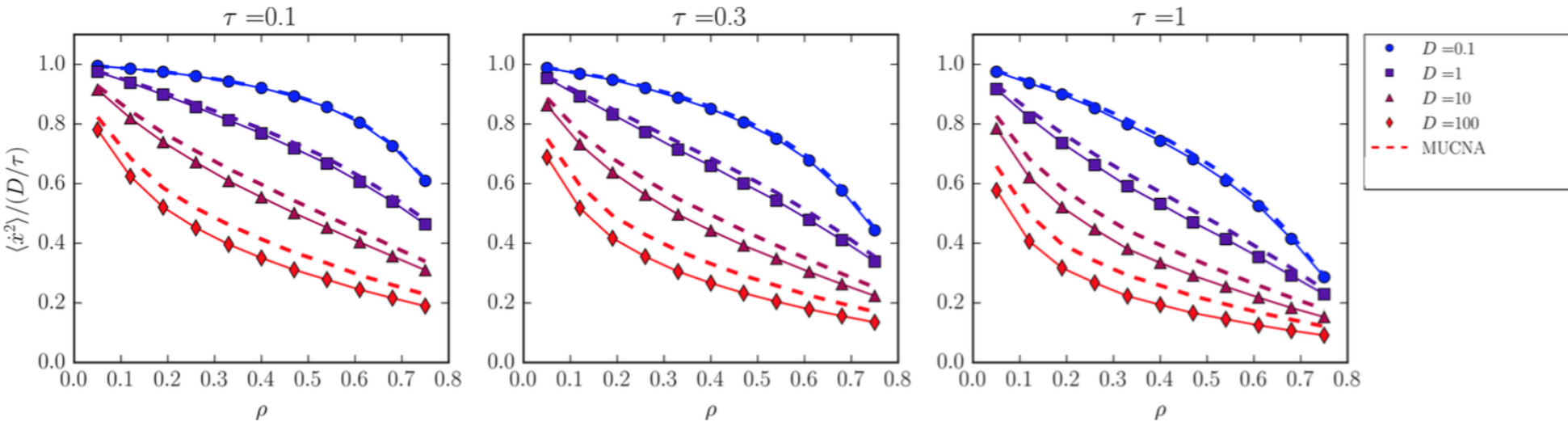
Testing the $\Pi(v)$ only

$$\langle \dot{x}^2 \rangle = N^{-1} \left\langle \int d\dot{\mathbf{x}}\, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}}\, \mathcal{N}^{-1} e^{-\tau/(2D)\dot{\mathbf{x}}\cdot[\mathbf{I}+\tau\nabla\nabla\phi]\cdot\dot{\mathbf{x}}} \right\rangle_{\text{num confs}}$$



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Key questions and results

How do we interpret the normalisation factor Z: Free energy?

$$F \stackrel{?}{=} -T \ln Z$$

$\mathcal{F}[P] = TrP(\mathcal{H} + \mathcal{T} \ln \mathcal{P})$ for all normalised distribution one has the following H-theorem

$$\frac{d\mathcal{F}}{dt} \leq 0. \tag{15}$$

How the $-T \ln Z$ is related to thermodynamic observables? Pressure:

$$p \stackrel{?}{=} T \frac{\partial \ln Z}{\partial V}$$

Does it coincides with the mechanical pressure: force on a wall? Virial pressure. To first order in τ, yes, virial and "thermodynamic" pressure coincide.

$$\partial_t P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N; t) = \mathcal{L}_{FP} P_N(\mathbf{r}_1, \ldots, \mathbf{r}_N; t) \tag{16}$$

$$\frac{d\langle O(t)\rangle}{dt} = \int d^N\mathbf{r} P_N \sum_{\alpha i} \sum_{\beta k} M^{-1}_{\alpha i,\beta k} \Big(\frac{1}{\gamma} F_{\beta k} \frac{\partial}{\partial r_{\alpha i}} + D \frac{\partial}{\partial r_{\alpha i}} \sum_{\gamma j} M^{-1}_{\gamma j,\beta k} \frac{\partial}{\partial r_{\gamma j}} \Big) O \tag{17}$$

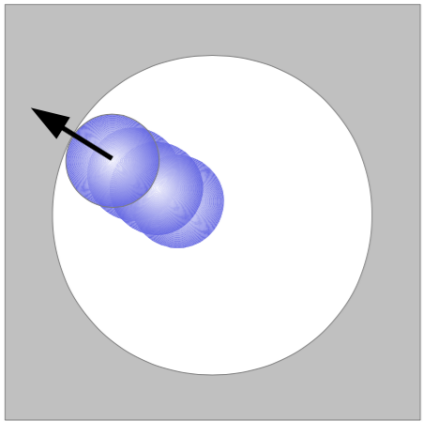
$$O = \sum_{\alpha i} \Big(\frac{r^2_{\alpha i}}{2} + \frac{\tau}{\gamma} \frac{\partial}{\partial r_{\alpha i}} r_{\alpha i} \Big) - \frac{\tau}{\gamma} \tag{18}$$

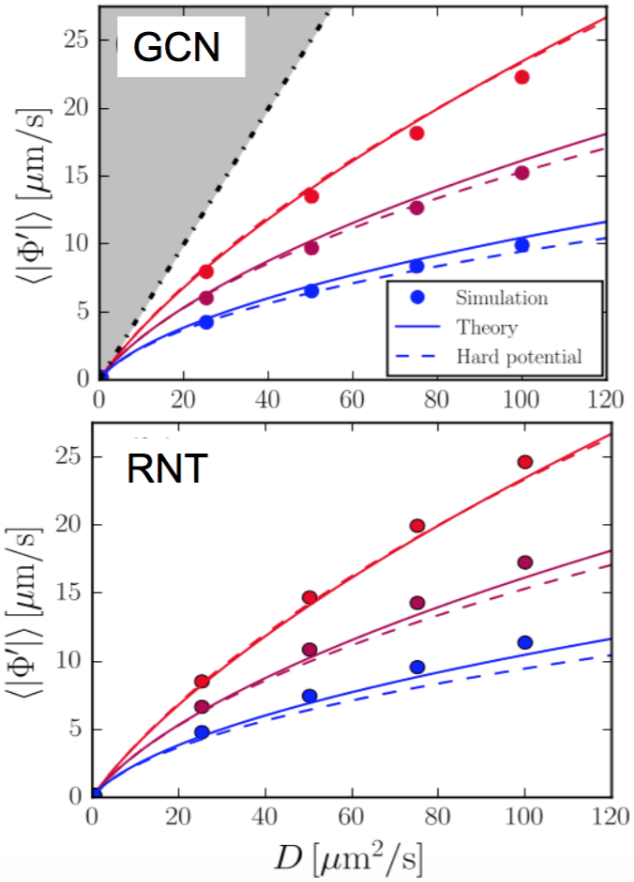
$$\sum_i^N \langle (F_i^{ext} + F_i^{int}) \cdot \mathbf{r}_i \rangle + D\gamma \sum_{\alpha i} \langle M^{-1}_{\alpha i,\alpha i} \rangle = 0 \tag{19}$$

The forces exerted by the bounding walls of the container, represented by the first term are macroscopically described as external pressure: each oriented area element $d\mathbf{A}$ exerts a force $-p_v(\mathbf{r})d\mathbf{A}$ (the subscript "v" stands for virial) so that

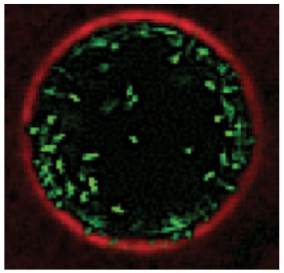
$$\sum_i^N \langle F_i^{ext} \cdot \mathbf{r}_i \rangle = - \oint p_v(\mathbf{r}) \mathbf{r} \cdot d\mathbf{A} = -\bar{p}_v V d \,, \tag{20}$$

Pressure at a circular wall





...but very similar pressure again!
Do we see this in experiments?



I. D. Vladescu et al. *PRL* **113**, 268101 (2014)

Future directions

Understand phase behaviour and phase transitions (if any) between stationary bulk phases .
Recall mechanism of attraction out of repulsion.
So far, only numerical results.
Mean field theory is possible, but the range of effective interactions is so short that it cannot be trusted quantitatively.
Explore non stationary regime.
Go beyond the Unified color approximation.

- U.Marini Bettolo Marconi and C. Maggi, Soft Matter **11** (45), 8768-8781 (2015).
- C. Maggi, U.Marini Bettolo Marconi, N. Gnan and R. Di Leonardo, Scientific Reports **5**, 1-7 (2015).
- U.Marini Bettolo Marconi, N. Gnan, C. Maggi, M. Paoluzzi and R. Di Leonardo, Scientific Reports (2016).