Self-propulsion through symmetry breaking

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Solvay Workshop - "Bridging the gaps at the PCB interface"
Multiscale Modelling in Physics, Chemistry and Biology

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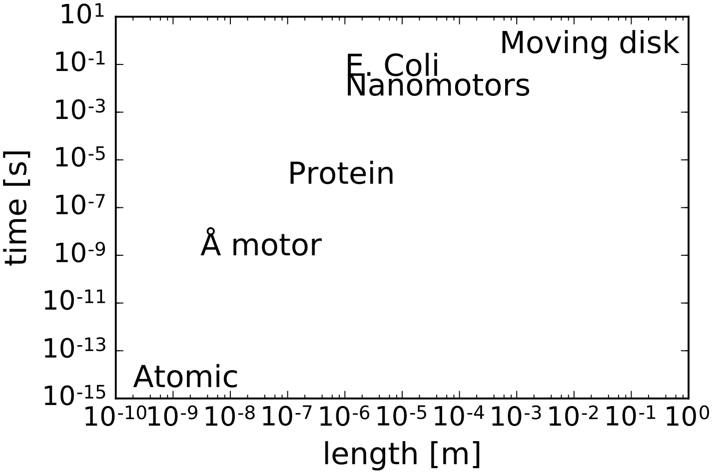
http://pdebuyl.be/

Active colloids

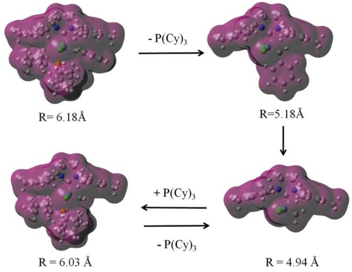
- Microscopic algae Volvox carteri from Raymond E. Goldstein group, Phys. Rev. Lett. **105**, 168101 (2010), about 200 μm
- Bacteria, μm scale
- Enzymes, nm scale
- Nanomotors, nm to μm scale
  - Theory: R. Kapral, J. Chem. Phys. **138**, 020901 doi:10.1063/1.4773981
  - Experiments: S. Ebbens, Cur. Opinion Coll. Interf. Sci. **21** 14 (2016) doi:j.cocis.2015.10.003

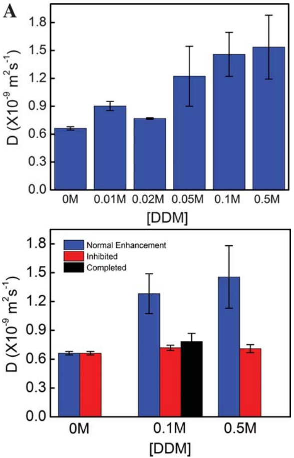
Scales



Moving disk
E. Coli
Nanomotors
Protein
Å motor
Atomic
time [s]
length [m]
10^1
10^-1
10^-3
10^-5
10^-7
10^-9
10^-11
10^-13
10^-15
10^-10 10^-9 10^-8 10^-7 10^-6 10^-5 10^-4 10^-3 10^-2 10^-1 10^0

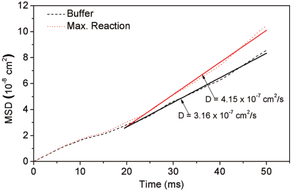
Enhanced diffusion of Grubbs' catalyst

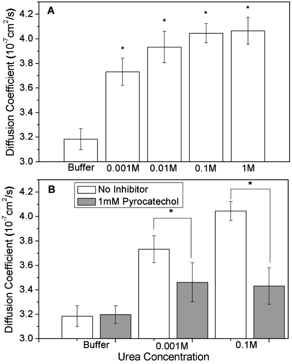




- Pavlick *et al* Nanoscale (2013) – Group of Ayusman Sen, PSU
  doi:10.1039/C2NR32518G

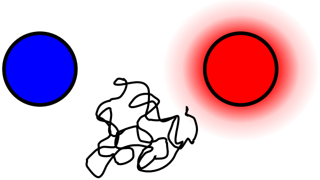
Enhanced diffusion of Urease





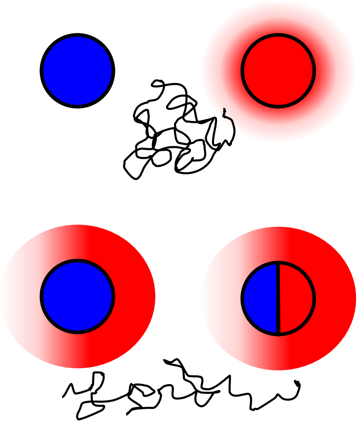
- Urease picture from Wikipedia page on Urease.
- Muddana *et al*, JACS (2010) doi:10.1021/ja908773a

Operation of active colloids



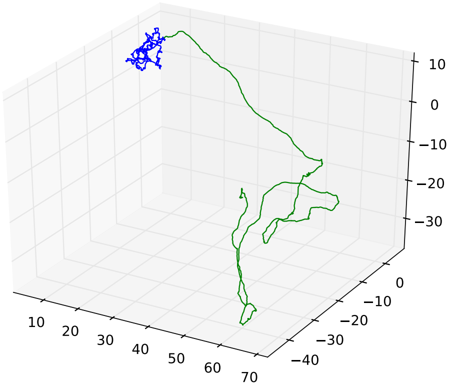
- Blue = passive   Red = active

Operation of active colloids



- Blue = passive   Red = active
- Functionalize specific sites of a colloid.
- Asymmetry → gradient generation.
- → self-propulsion.
- Basic operation of a chemical engine.

Equilibrium and active trajectories



A word on the method

- Multiparticle Collision Dynamics + Molecular Dynamics (Malevanets & Kapral, J. Chem. Phys. 1999 and 2000)[1]
- Chemical activity
  - Catalytic: similar to Rückner & Kapral 2007

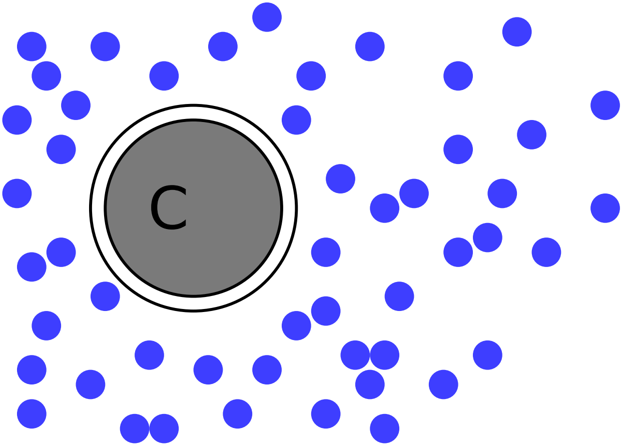
$$A + C \to B + C$$

  - Bulk: Reactive Multiparticle Collision Dynamics Rohlf, Fraser and Kapral 2008

$$B \to A$$

[1] Reviews: R. Kapral, Adv. Chem. Phys. **140**, 89 (2008), Gompper *et al* Adv. Polymer Sci. **221**, 1 (2008)

Principle of operation



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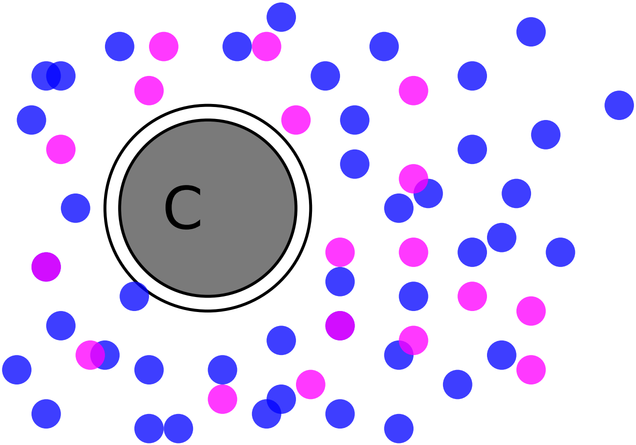
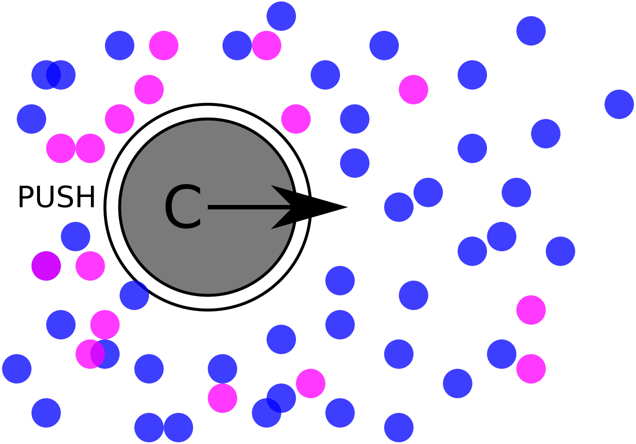


Principle of operation



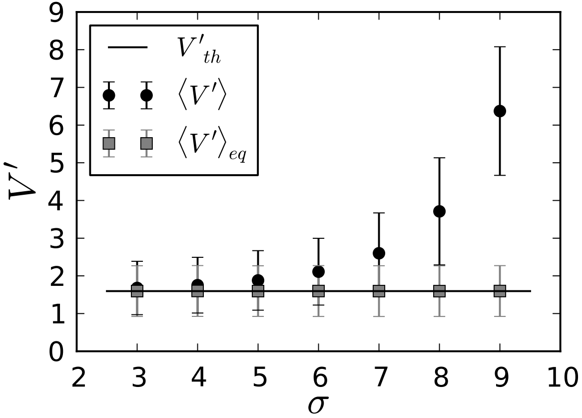
Dynamics of the active colloid

The departure of the dynamics from an equilibrium situation is tracked by the following quantities:

- The average speed $\langle V' \rangle$
- The distribution for the speed (norm of the velocity): $P(V')$
- The Mean Squared Displacement (MSD)
- σ is the radius of the colloid

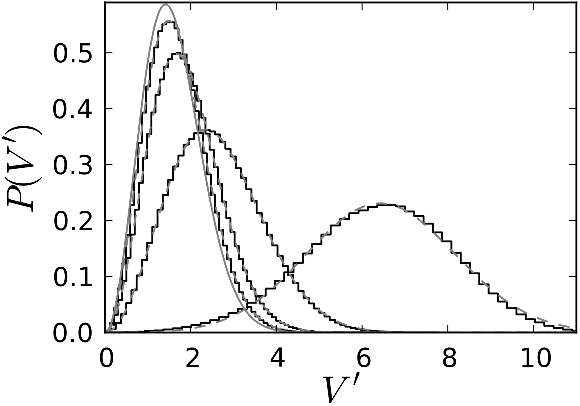
All speeds V' are scaled by the thermal velocity $\sqrt{\frac{k_B T}{M}}$, where M is the mass of the colloid.

Simulation Results: $\langle V' \rangle$



Simulation Results: $P(V')$

From left to right: $\sigma = 3, 5, 7$ and 9.



Simulation Results: raw data

Table: Speed distribution parameters, and ballistic and diffusive components of the MSD.

σ	3	4	5	6	7	8	9
$\langle V' \rangle$	1.7	1.8	1.9	2.1	2.6	3.7	6.5
V'_B	1.7	1.9	1.8	2.0	2.6	3.8	6.5
$D_C\ 10^3$	11.4	12.6	16.2	24.0	55.9	223.4	843.3
$D_C^N\ 10^3$	5.64	3.28	2.95	1.80	1.41	1.35	0.93

- V'_B ballistic component of the MSD

Predicting the onset of self-propulsion

$$\partial_t n_B(\mathbf{r}, t) = D\nabla^2 n_B(\mathbf{r}, t) - k_2 n_B + \mathcal{S}(\mathbf{r}, t).$$

- D is the diffusion coefficient of the fluid.
- k_2 is the bulk rate of the reverse reaction.
- $\mathcal{S}$ is the source term on the surface of the colloid that we approximate by a point source.
- Balancing against the friction, we obtain a condition for the threshold of the instability:

  $$\mathcal{C} = \frac{4\pi}{3} \frac{k_B T}{\zeta} \frac{R_0^2}{D^2} |\lambda^2| r_f,$$

  when $\mathcal{C} = 1$. ζ is the friction coefficient, λ is the Derjaguin length and r_f the reaction rate per unit area.

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- In the units of the simulations, the critical radius of the particle is $\sigma \approx 4.7$.

Conclusions

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- Demonstration of self-propulsion via flucluation induced symmetry-breaking
- Instability mechanism consistent with continuum picture
- Sub-threshold diffusion constant *not* equal to equilibrium one

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Paper

- PdB, A. S. Mikhailov and R. Kapral
  EPL **103**, 60009 (2013) - arXiv:1401.1360

Simulations

- See my poster and `https://github.com/pdebuyl-lab/RMPCDMD`
- Open-source, reproducible(?)

Simulation Results: raw data

Table: Speed distribution parameters, and ballistic and diffusive components of the MSD.

σ	3	4	5	6	7	8	9
V'_C	0.04	0.4	0.6	0.9	1.3	2.6	5.9
w	1.1	1.1	1.1	1.2	1.4	1.7	1.8
$\langle V' \rangle$	1.7	1.8	1.9	2.1	2.6	3.7	6.5
V'_B	1.7	1.9	1.8	2.0	2.6	3.8	6.5
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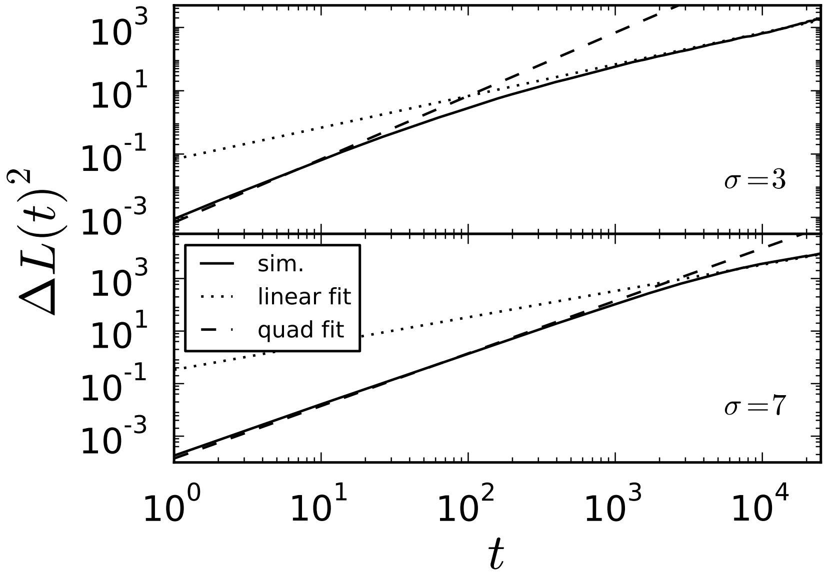
$$P(V') = \frac{1}{\sqrt{2\pi}w}\frac{V'}{V'_C}\left(e^{-(V'-V'_C)^2/2w^2} - e^{-(V'+V'_C)^2/2w^2}\right),$$

MSD



10^3
10^1
10^{-1}
10^{-3}
$\sigma = 3$
$\Delta L(t)^2$
sim.
linear fit
quad fit
10^3
10^1
10^{-1}
10^{-3}
$\sigma = 7$
10^0
10^1
10^2
10^3
10^4
t