CONTROLLING THE SHAPE OF CLUSTERS WITH A MACROSCOPIC FIELD

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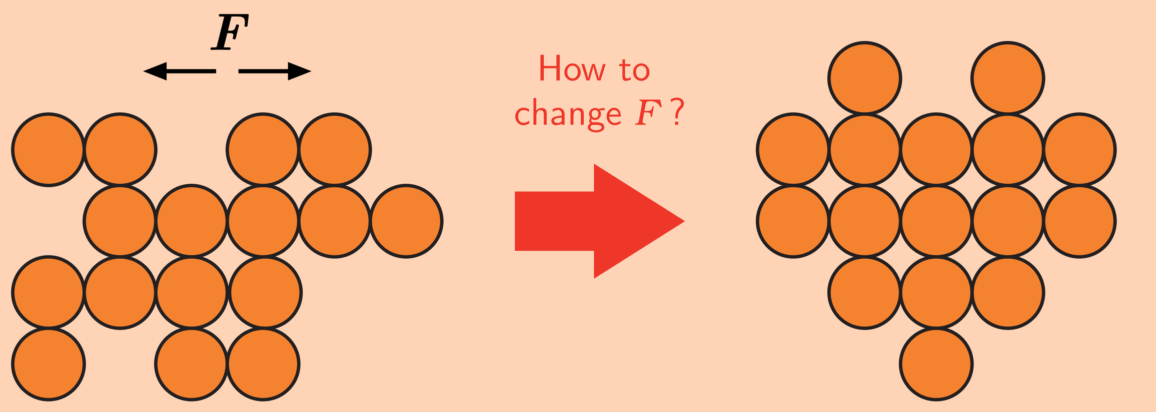
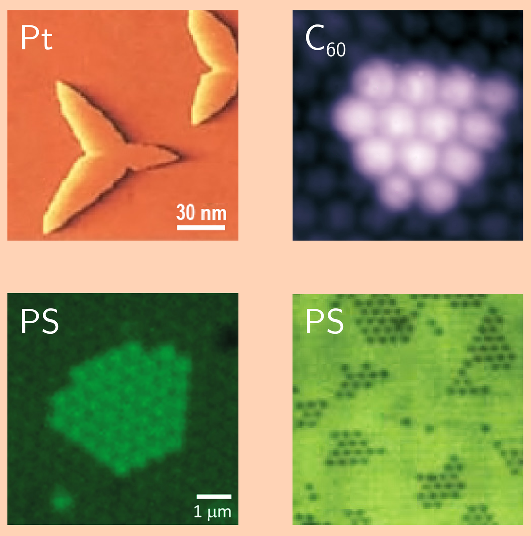
Idea: control of shapes in non-equilibrium clusters





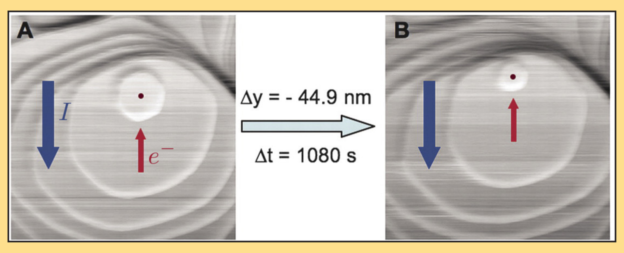
F = macroscopic control parameter
e.g.: electric field, temperature gradient....

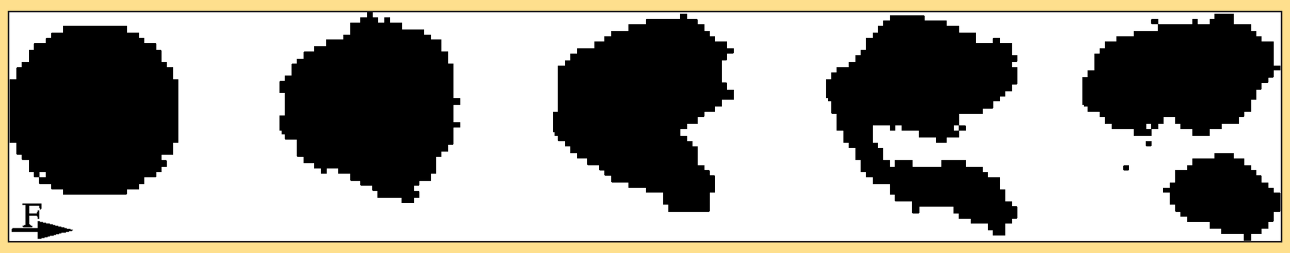
Islands, Mounds and Atoms, Springer (2004)
Sci. Rep. 4 (2014)
Crys. Growth Des. 18 (2018)
Science 327 (2010)

Case study: electromigration-driven islands

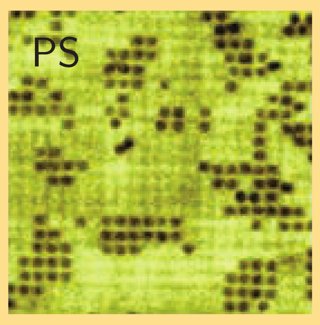
Electromigration: **current-induced mass transport** that arises from a momentum exchange between conducting electrons and island atoms.

Science 328 (2010)
Phys. Rev. B 62 (2000)
Science 327 (2010)

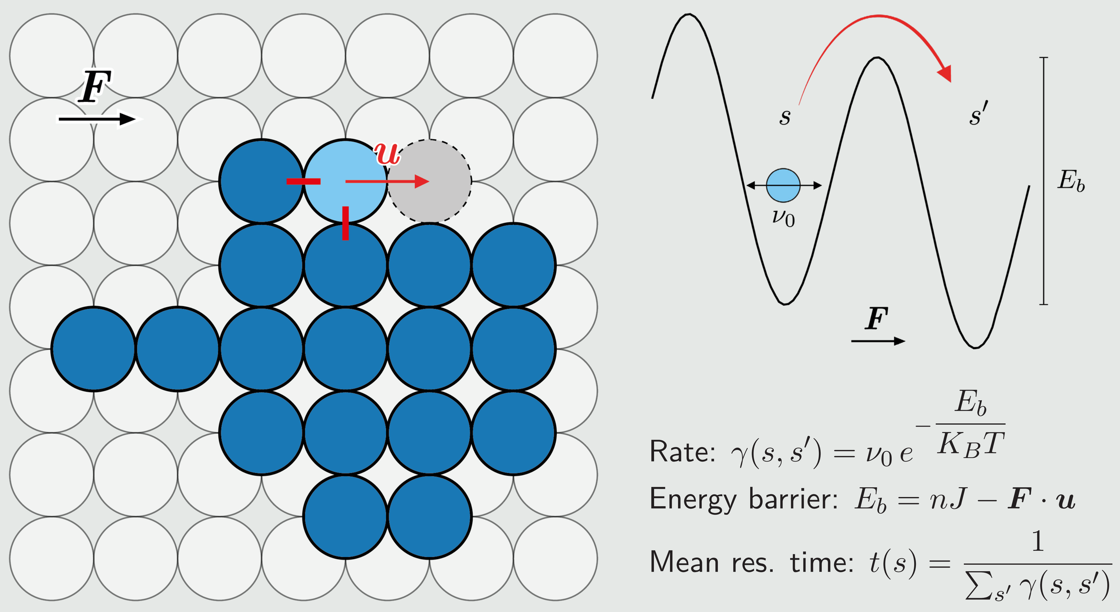




For colloids:
- Electrophoresis,
- Thermophoresis,
- Magnetic force...



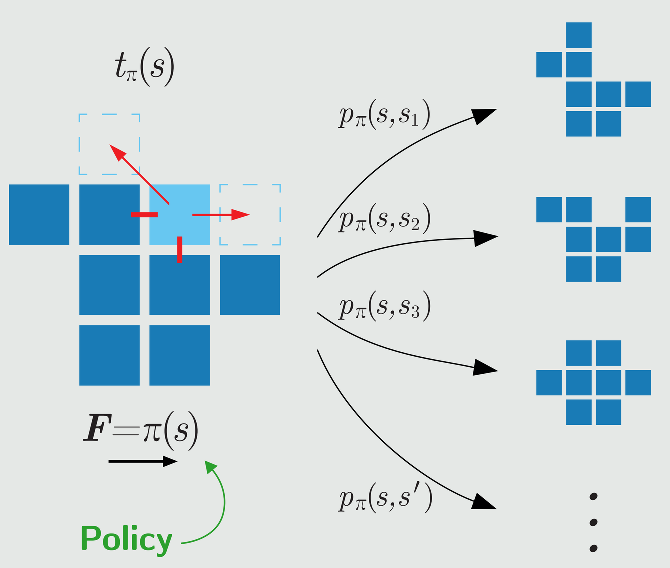
Model: lattice model



Rate: $\gamma(s,s') = \nu_0\, e^{-\frac{E_b}{K_B T}}$

Energy barrier: $E_b = nJ - \boldsymbol{F}\cdot\boldsymbol{u}$

Mean res. time: $t(s) = \frac{1}{\sum_{s'}\gamma(s,s')}$



- States: Island shapes
- Actions: $F_x = (-F_0, 0, F_0)$
- Rewards: $-t_\pi(s)$ (until target is reached)

Aim: minimize physical time to reach a given target

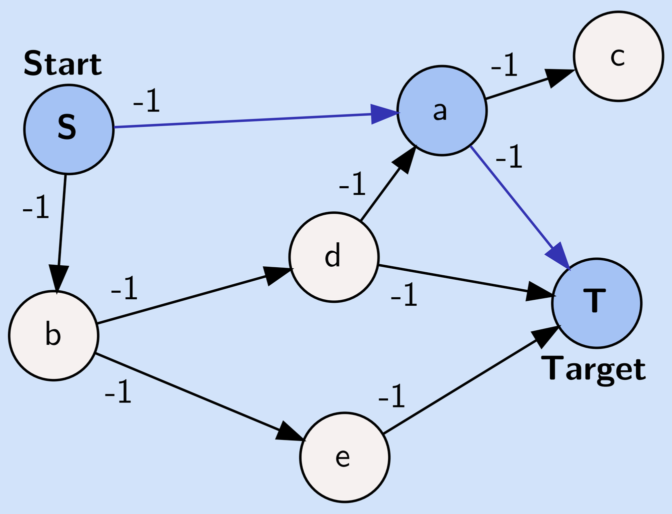
π_*

How to obtain the **optimal policy** to control the cluster?

Method 1: Dynamic Programming (DP)

Compute the optimal policy on the state space. This problem can be seen as the optimization of the first passage time on the graph of the dynamics.

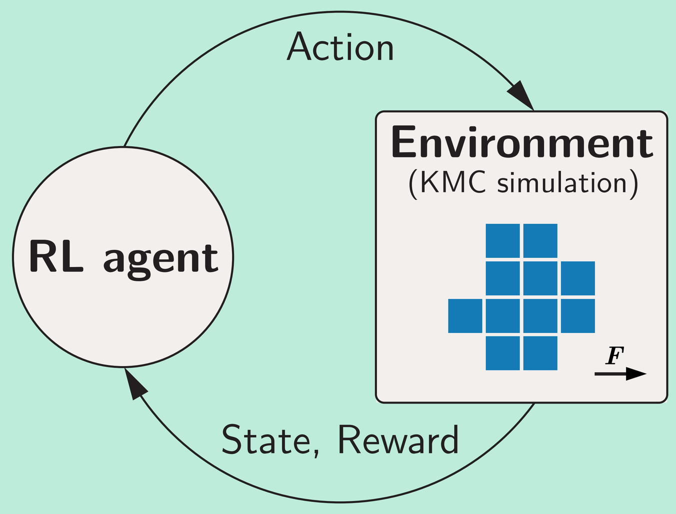
Requires **complete knowledge** of the governing laws of the environment.



Method 2: Reinforcement Learning (RL)

Learn from experience and find the optimal policy. This method is closer to what could be done in an experiment.

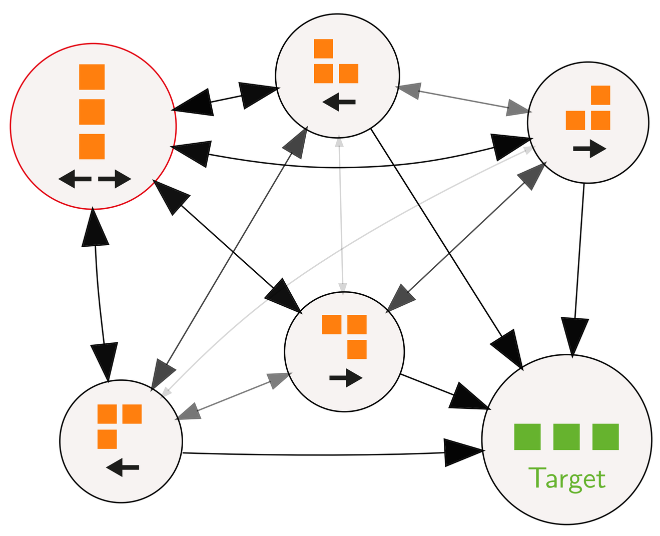
Requires **continued observation** of the evolution of the environment.



DYNAMIC PROGRAMMING

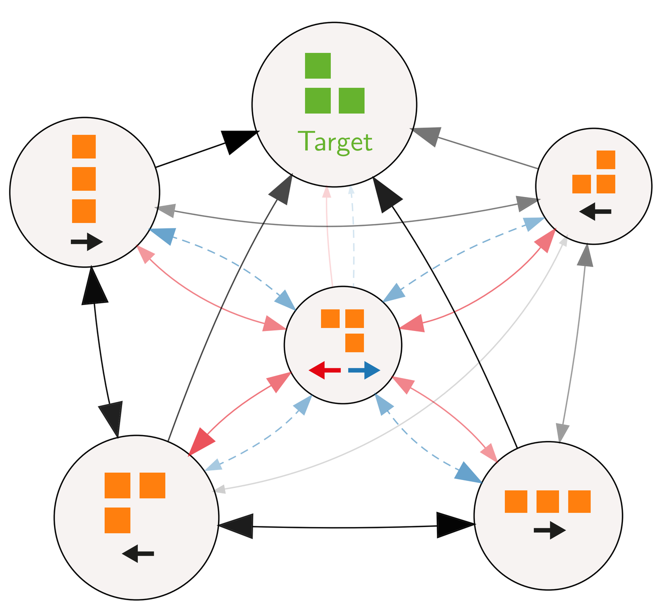
Degeneracy of π_*

Due to the symmetry of the target, the optimal action on the red state is **not unique**.

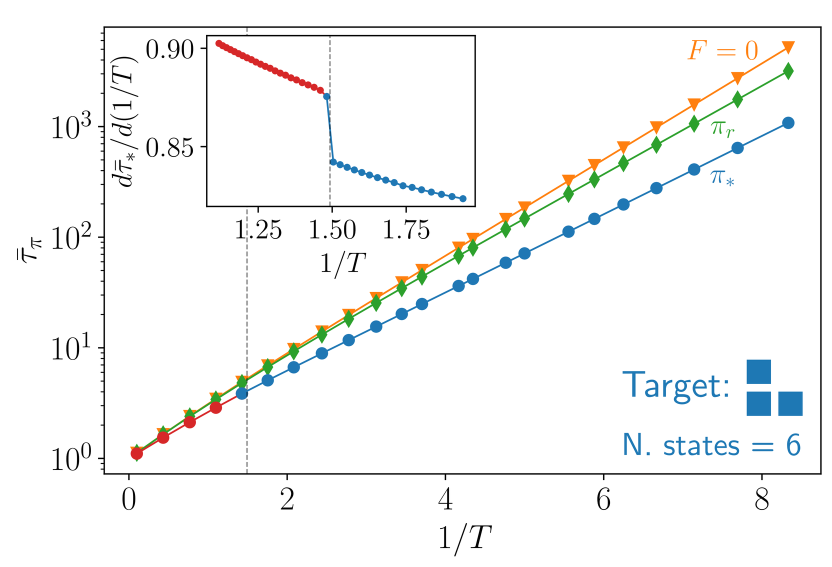


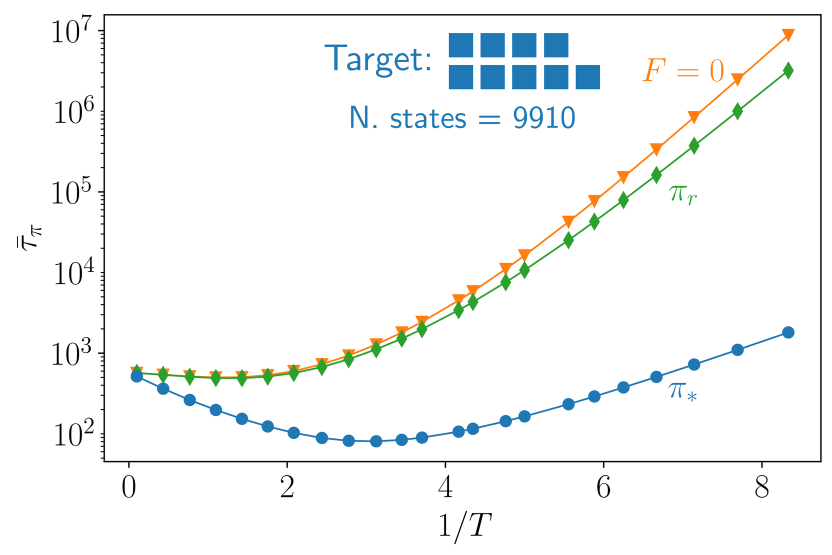
Discontinuity of $\pi_*(T)$
($T = 0.66$, $T = 0.67$)

The optimal action on the state in the center of the graph **switches** from right to left when increasing the temperature.



Expected return time to target





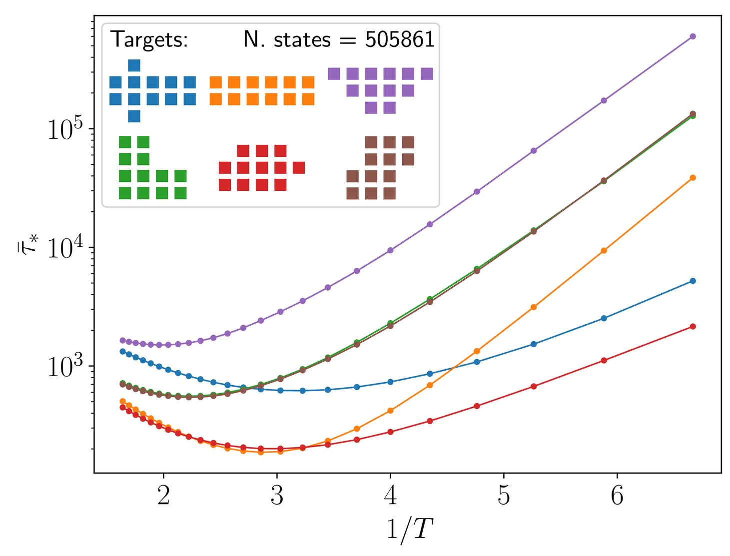
We **can** do better than the unbiased environment or a random policy!

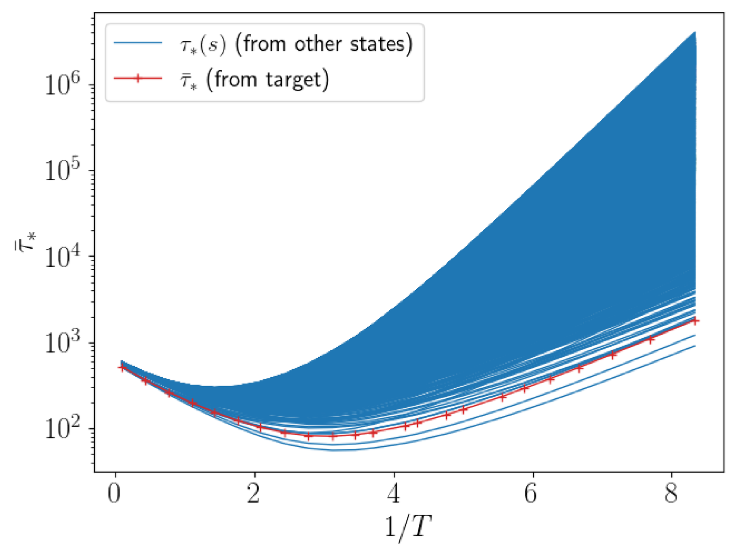
The transition in $\pi_*(T)$ leaves a trace in the first derivative of the optimal return time to target appears.

When we consider a bigger target, a **minimum** in the optimal expected return time to target appears, implying that there is a temperature at which the control of the cluster shape is optimal.

This is not specific to this target but it is a **common feature** that appears as we consider targets of increasing size.

The minimum is not only observed in the return time to target, but also when starting from **other states** in the system.

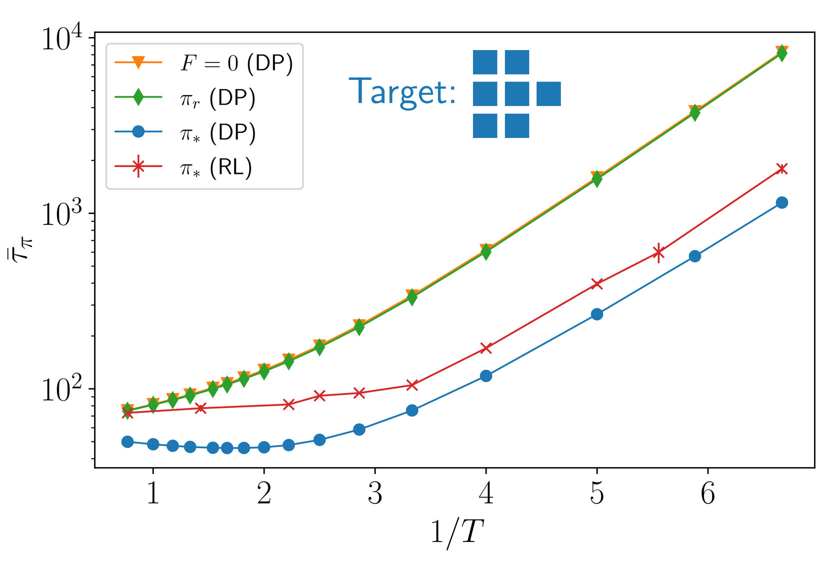




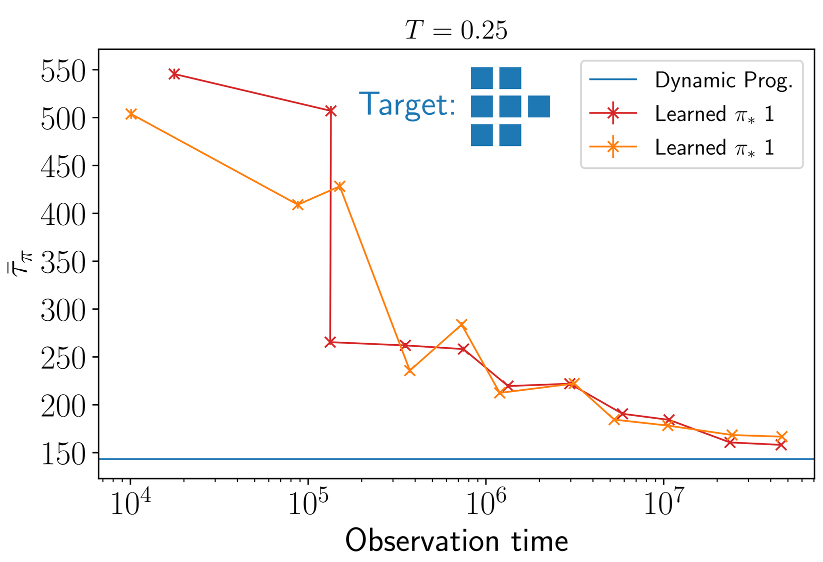
REINFORCEMENT LEARNING

We **can** learn a policy by observing the environment! This policy is still better than the unbiased environment or a random policy, but not as efficient as the optimal policy computed with DP.

At high temperatures, learning is difficult because of **thermal fluctuations**.



By increasing the **observation time** of the environment, the optimal policy learned by the RL agent approaches the performance of the one computed with DP.



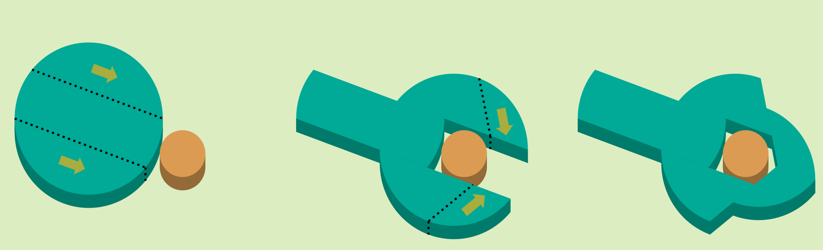
Perspectives

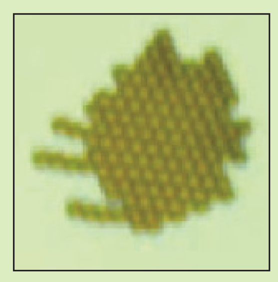
Experimental application on colloids seems quantitatively reasonable.

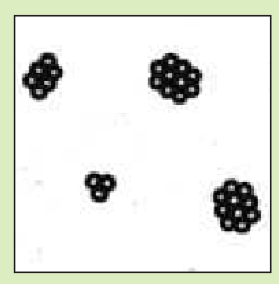
Consider **non mass-preserving** processes.

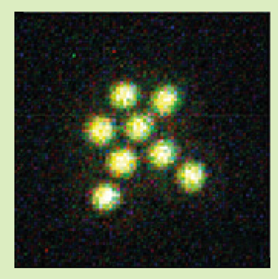
Consider **other models** to describe different interactions:
- Magnetic interactions
- Acoustic interactions (Bjerknes force)
- Interactions with light (optical binding)

Functional **metamaterials** (colloidal robots):









Langmuir 26 (2010)
Phys. Rev. Lett. 106 (2011)
J. Phys. Chem. Lett. 9 (2018)
PNAS 118 (2021)