Non-conservative forces & effective temperatures in active matter

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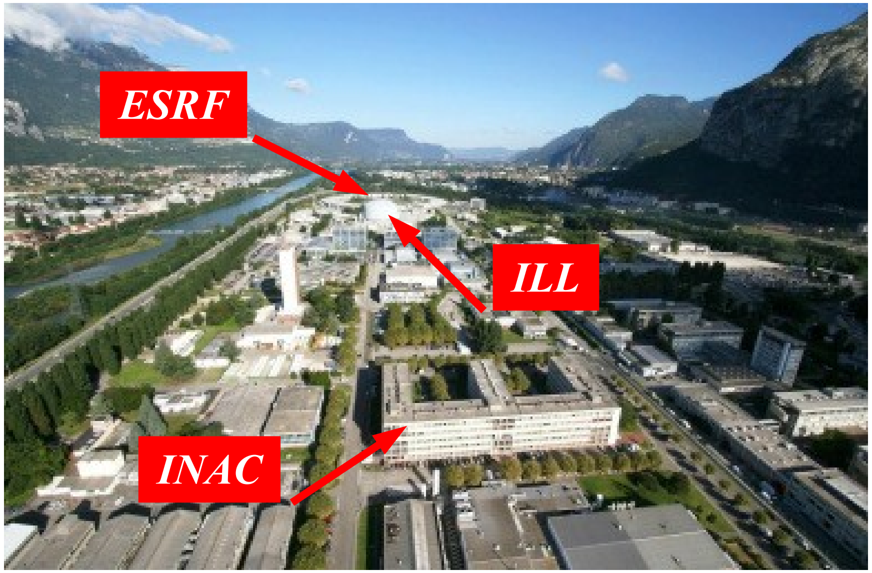
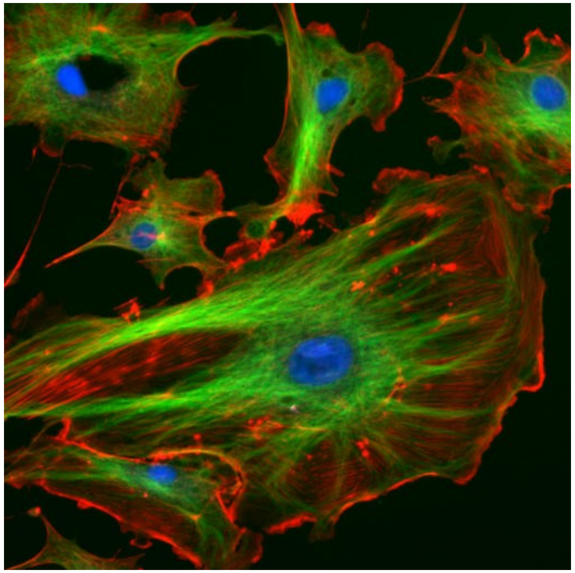




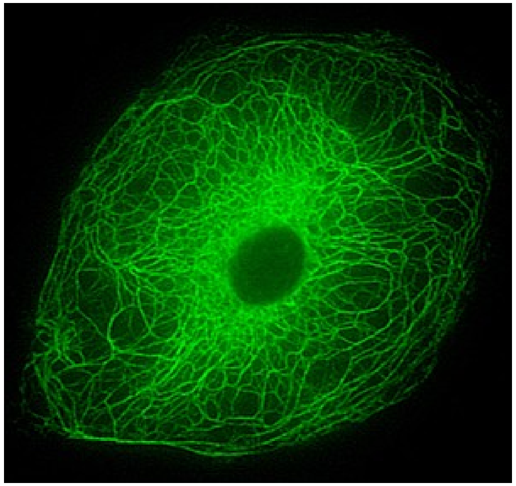
Very interesting objects: the active matter

- Active matter **absorbs energy** from the environment or **internal** fuel tanks and use it to carry out motion
- Energy is partially transformed into **mechanical work** and partially dissipated in form of **heat**
- Units interact **directly** or through **disturbances** propagated in the medium
- **Conservative forces** and **thermal fluctuations** are complemented by **non-conservative forces**
- Many examples: highly deformable **soft** solids, viscoelastic fluids... (**biological**/**non-biological** origin)

µm - length scales - m

images from WikiPedia

cytoskeleton



bacterial suspensions

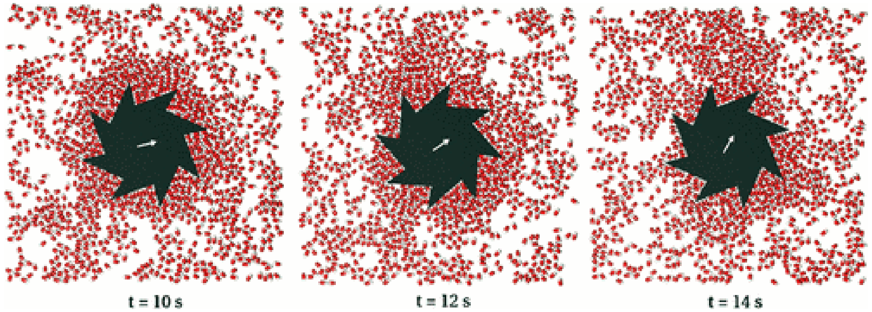
swarms of animals

Active matter can generate motion at mμ scale

- **Asymmetric** motors propelled by a bath of bacteria

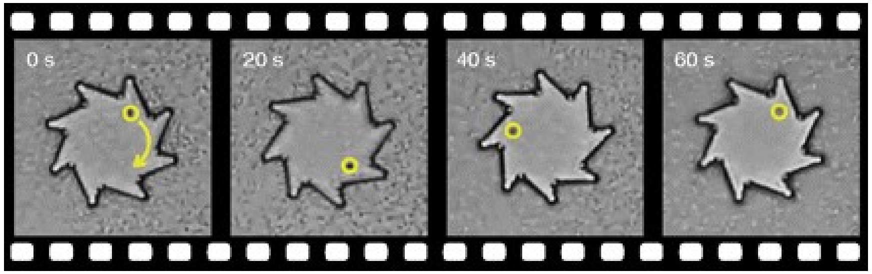
First, simulation *(L. Angelani et al. 2009)*:

net rotary counterclockwise motion of the gear



Next, experiment *(R. Di Leonardo et al. 2010)*:

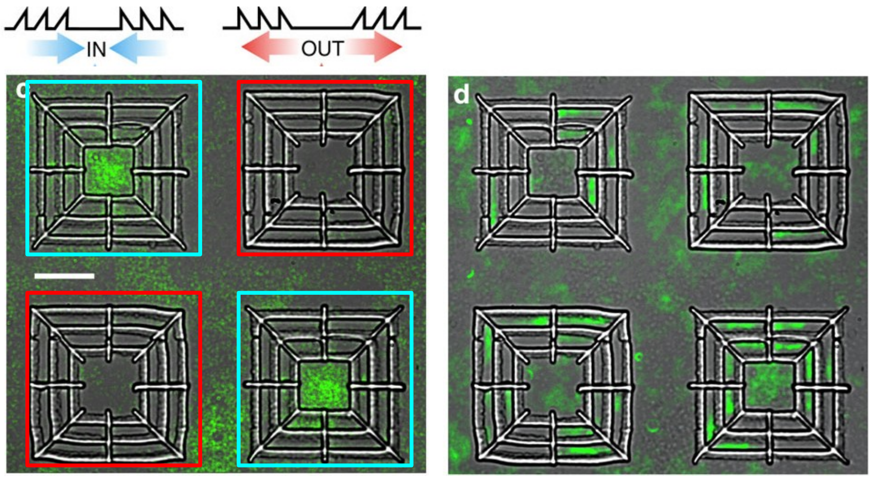
Rotating micro **saw-toothed** disks in **E. coli**



- Targeted **delivery** of colloids **by swimming bacteria**

3-dim microstructures define accumulation areas

where bacteria **spontaneously** store colloidal particles



with bacterial bath **without** bacterial bath

(N. Koumakis et al. 2013)

Much room for statistical mechanics

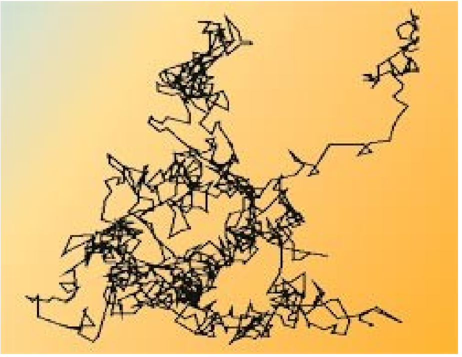
- Active (**self-propelled**) matter is kept in a **non-equilibrium steady state**
- The difference with other more classical driven systems is that the energy input is located on **internal units** (motors) not at **boundaries of the sample** (sheared fluids, vibrated granular media)
- Interesting features: out-of-equilibrium phase transitions, self-organization, collective motion, unusual mechanical properties, very large fluctuations...

  - Which thermodynamic concepts can be applied to active matter?
  - Can we “stand on the shoulders” of giants who developed **glassy physics**?
  - In **passive** glassy systems **effective temperature** T_{eff} is an interesting concept...

Equilibrium fluctuation-dissipation theorem

- Many-body dynamics very complicated, but at **thermodynamic equilibrium**...
- We can forget about dynamics and choose a **statistical** description in terms of **T**, **S**, etc...
- But: thermodynamics still contains information on dynamics

brownian motion



- Energy **gained** through fluctuations
- Energy **lost** through dissipation (viscous drag)

$$\xi = \frac{k_B T}{m D}$$

ξ friction coefficient

D diffusion coefficient

T temperature

At equilibrium response & correlation are **not** independent: **Fluctuation-Dissipation Theorem**

$$E_o(C) \rightarrow E_\epsilon(C) = E_o(C) - \epsilon B(C)$$

$$\chi_{AB}(t) = \lim_{\epsilon \rightarrow 0} \left(\frac{1}{\epsilon}\right) \left(\langle A(t) \rangle_\epsilon - \langle A \rangle_o \right) = \frac{1}{k_B T} \left[C_{AB}(0) - C_{AB}(t) \right]$$

Integral form

→ Note that we can **measure** T from a **parametric plot** of χ vs C ...

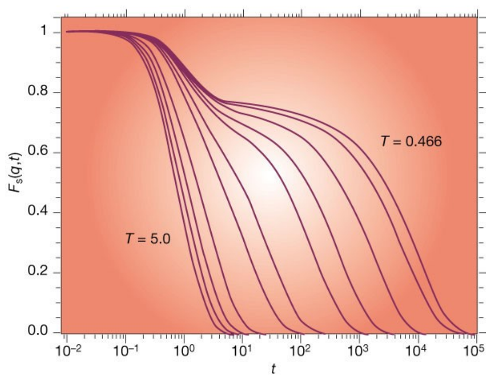
Out-of-equilibrium Fluctuation-Dissipation relation

- Question: Is it possible to measure a **temperature** in **out-of-equilibrium** conditions?
- Answer: **Yes**, but we need a **suitable thermometer**… *(J. Kurchan 2005)*
- An **harmonic oscillator** of frequency ω coupled to an observable A "reads" a temperature:

- **equilibrium** $T = \frac{2}{k_B} \langle K \rangle$ **heat-bath** temperature (equipartition)
- **out-of-equilibrium** $T_{eff}(\omega, A) = \omega \frac{\Re[C(\omega, A)]}{\Im[R(\omega, A)]}$ **effective** temperature of A at timescale ~ **1/ω**

Example: supercooled liquids & glass formation

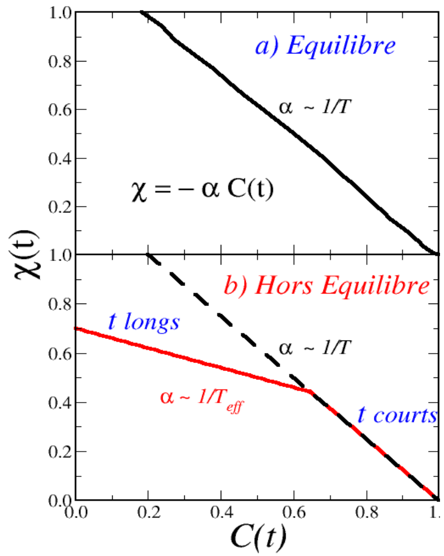
(**well-separated** time-scales $\tau_{fast} << \tau_{slow}$)



A thermometer of frequency ω reads

$$\rightarrow \begin{array}{ll} T & \omega \gg 1/\tau_{slow} \\ T_{eff} & \omega \sim 1/\tau_{slow} \end{array}$$

with $T_{eff} > T$



Similar results observed in analytical **models**, **simulations** and (possibly) **experiments**...

Our scientific question: T_{eff} for active matter?

- In **equilibrium**, correlations and response to a perturbation are related by temperature (**FDT**)
- A suitable **thermometer** can be defined which measures the same temperature everywhere (**tracer**)

- In **out-of-equilibrium**, FDT holds in a *generalized* form (**FDR**)
- A well-tuned thermometer measures (at least) two temperatures: T for **fast** modes, T_{eff} for **slow** modes
- Theoretical, numerical and experimental evidences for **external** perturbations (T or P jumps, shear,...)

Our questions:

- What happens in **active self-propelled soft matter**, with **internal (non-conservative) stimuli**?
- Can the concept of **effective temperature** help?
- Can effective temperatures be **measured**?
- Can we establish a **direct correlation** between T_{eff} and the level of **activity**?

The tool: molecular dynamics simulations

A Molecular Dynamics simulation is a true, **in-silico** experiment:

- Choose your sample and level of description (**modeling**)
- **No** additional hypothesis, **only physics rules**
- Let the system evolve in controlled conditions (**production**)
- Calculate observables (**analysis**)

1. Put your components in a simulation **box**

2. Integrate numerically the coupled **equations of motion**

3. Produce realistic equilibrium configurations ***{r,v}***

4. Use configurations to **directly calculate** observables

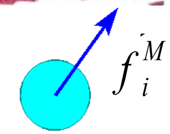
$$\vec{F}_i = -\vec{\nabla} \sum_{j \neq i} V(r_{ij}) + \vec{F}_{i,NC}$$

$$m_i \dot{\vec{v}}_i = -\xi m_i \vec{v}_i + \vec{F}_i + \vec{\eta}_i$$
$$\langle \vec{\eta}_i(t) \cdot \vec{\eta}_i(t') \rangle = 2 \xi m_i T \delta(t - t')$$

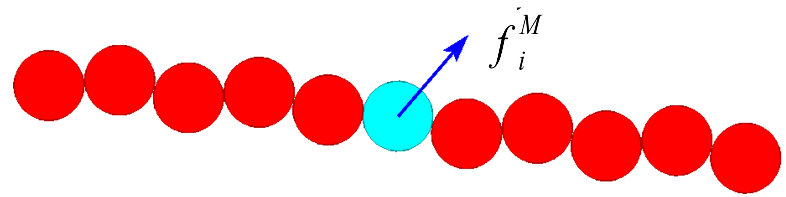
over-damped Langevin equation

Our toy models

- **1. Self-propelled particles**



- **2. Active semi-flexible polymers**



$$\vec{F}_i = \sum_j \vec{f}_{ij}^{inter} + \left(\sum_j \vec{f}_{ij}^{intra}\right) + \vec{f}_i^M$$

forces

$\vec{f}_{ij} = -\vec{\nabla}_i U$ — two-body conservative (Lennard Jones)

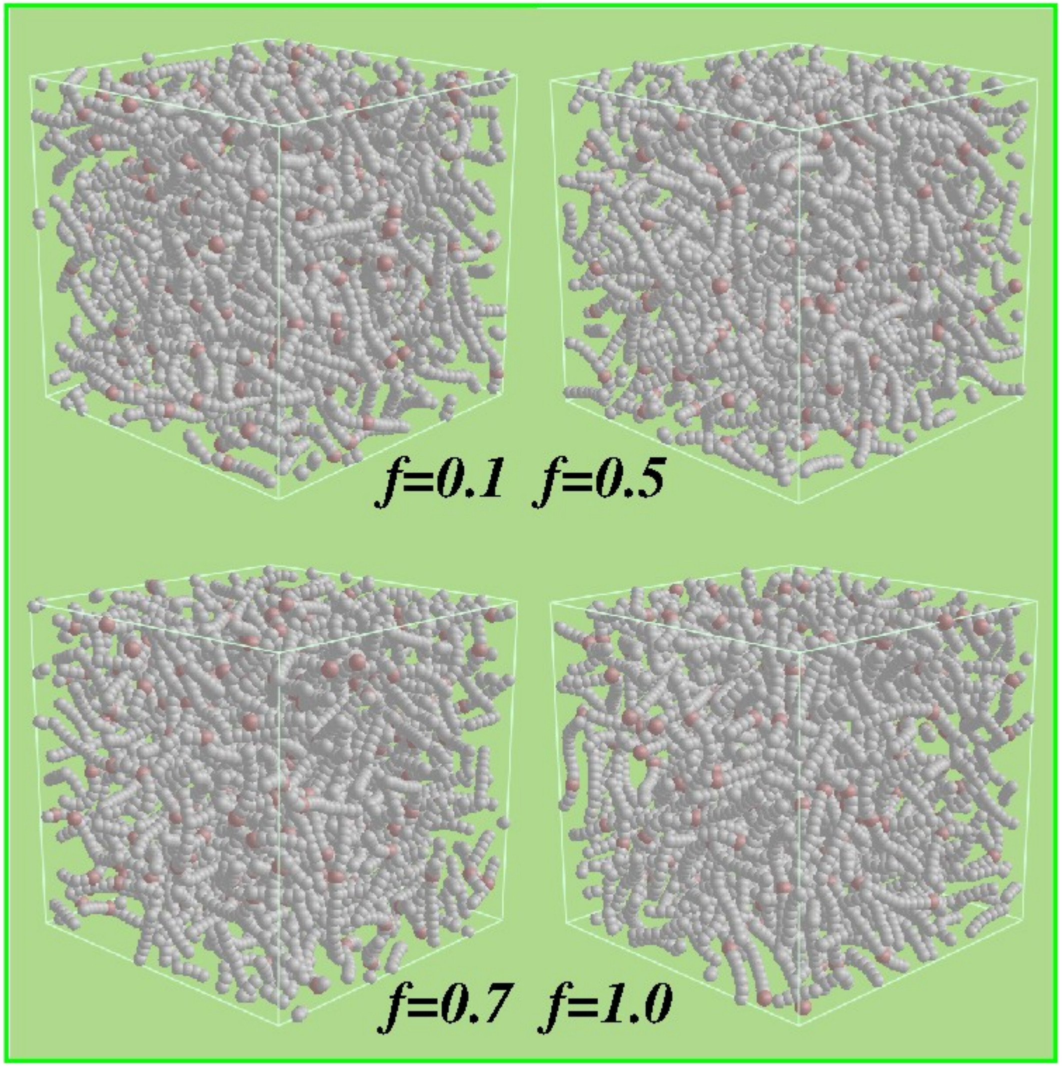
$\vec{f}_i^M$ — non-conservative **stocastic motor** forces (N_M, f_M, $\mathbf{n}_M$, τ_M)

the motor

- During $\boldsymbol{\tau}_{\mathbf{M}}$ **steps** independent **forces** are applied to N_M motorized (fixed, central) monomers
- The strength f_M is the same for all, the direction $\mathbf{n}_M$ is random and isotropic (**no preferential flow**)
- The subset of propelled monomers and $\mathbf{n}_M$ changes at each **power stroke**

Let's start by checking if the effect of activity (f_M) is non trivial (focus on polymers)...

System snapshots

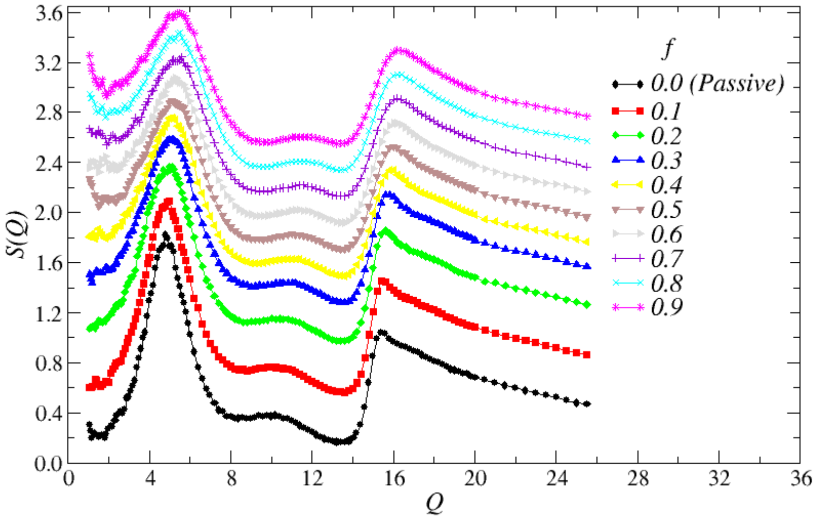


passive beads

motorized beads

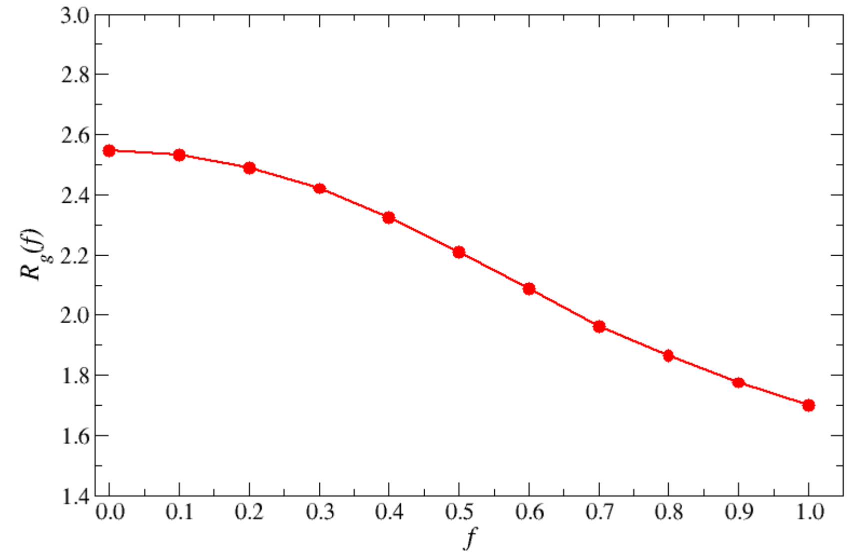
Not much can be said by visual inspection...

Active polymers: structure



Static Structure Factor

$$S(Q)=\frac{1}{N}\sum_{1=1}^{N}\langle|\rho(\boldsymbol{Q},t)|^2\rangle$$



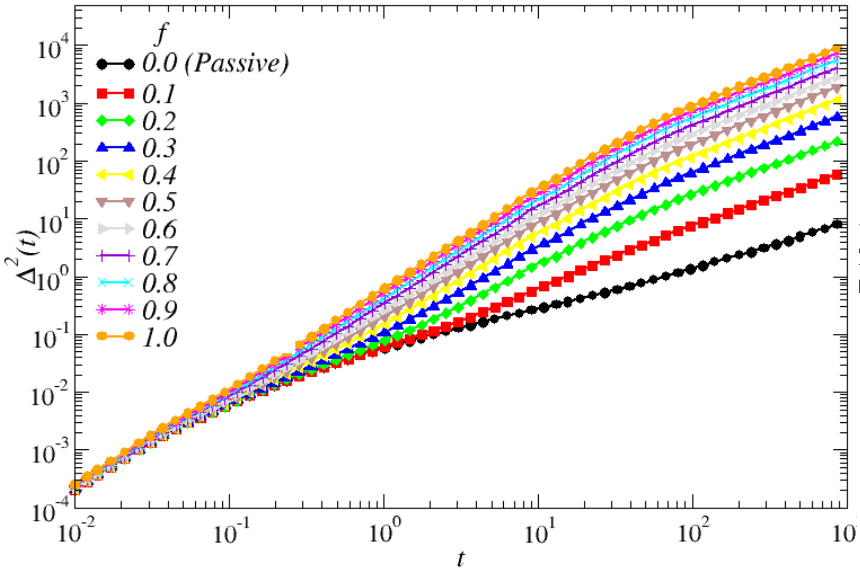
Radius of Gyration

$$R_g^2=\frac{1}{2N^2}\sum_{i\neq j}\langle|\boldsymbol{r}_i-\boldsymbol{r}_j|^2\rangle$$

- First maximum in S(Q) shifts to **higher Q**, nearest neighbors distances decrease - **crowding**
- Radius of gyration decreases, chains fold – **folding**
- Motor activity pushes **closer** the filaments which, at the same time, fold substantially
- Remember that we are working at **constant** external temperature (T_{bath}) and density

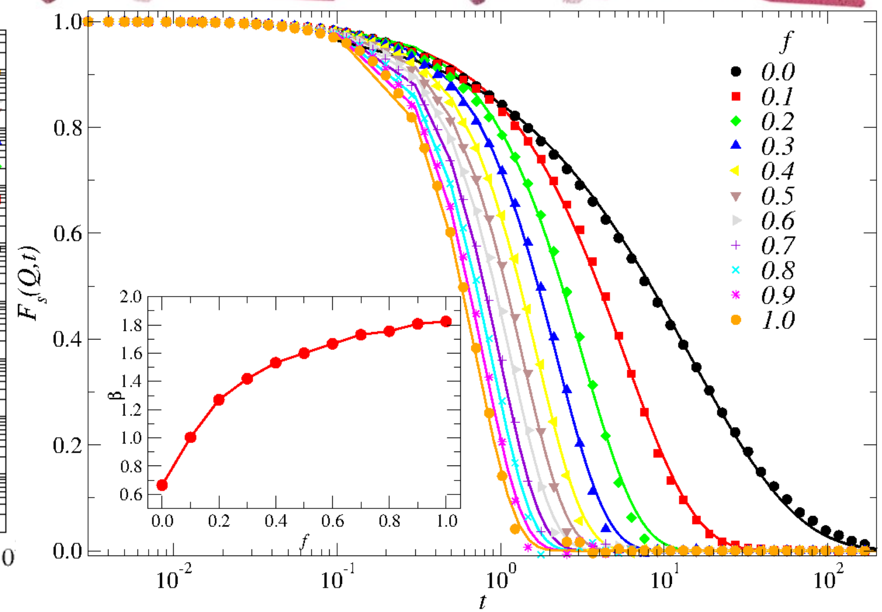
→ Effects on structure must couple to important effects on dynamics...

Active polymers: dynamics I



Mean-squared displacement

$$\Delta^2(t) = \frac{1}{N} \langle \sum_i |\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0)|^2 \rangle$$



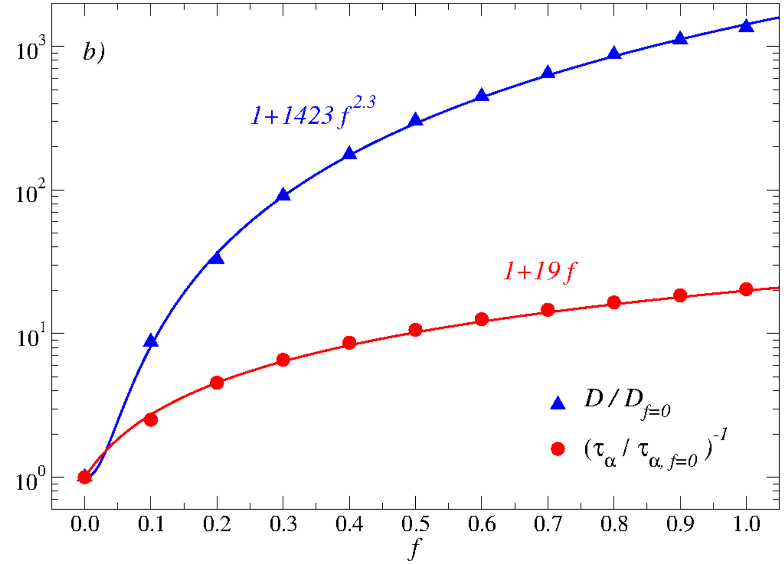
Self intermediate scattering function

$$F_s(Q,t) = \frac{1}{N} \langle \sum_i e^{i\boldsymbol{Q}\cdot[\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0)]} \rangle$$

From these data we can extract:

- **diffusion** coefficient $\quad D(f) = \lim_{t\to\infty} \Delta_f^2(t)/6\mathrm{t}$
- **α-relaxation** time $\quad F_s(Q,t) \propto \exp-(t/\tau_{\alpha f})^{\beta_f}$

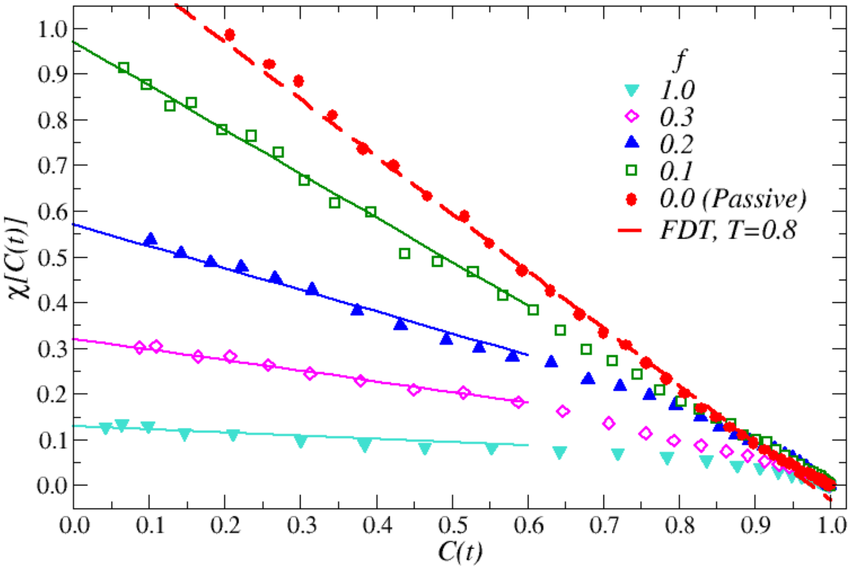
Active polymers: dynamics II



- Collective dynamics of filaments gets **faster under stronger f**
- Folding of filaments seems to **solve** local topological constraints and decrease **entanglement**...
- Similar dependence for active colloidal particles, with **f** replaced by **Peclet number** $P_e = \frac{v\,R}{D_o}$

  - Activity alters structure and dynamics of the passive system, at **fixed external conditions**
  - What happens in active states to **correlations and responses** of well chosen observables?

Effective temperatures I: correlation-response



Calculations are very intensive...

$$H_\epsilon = H_o - \epsilon B \qquad \chi_{AB}(t) = \frac{1}{T_{eff}(t)}[C_{AB}(0) - C_{AB}(t)]$$

$$A(t) = 1/N \sum^{N} \epsilon_i e^{i\vec{q}\cdot\vec{r}_i(t)}$$

$$B(t) = 2\sum^{N} \epsilon_i \cos[\vec{q}\cdot\vec{r}_i(t)]$$

$$P(\epsilon_i) = 1/2[\delta(\epsilon_i + 1) + \delta(\epsilon_i - 1)]$$

(L. Berthier and J.-L. Barrat 2002)

- **Trick:** A and B such that the good correlation function is $F_s(Q,t)$ (calculated in equilibrium)
- Follow the linear response of A when B perturbed (**several** instances of the perturbation field)
- Measure T_{eff} by calculating the long-time slope of the parametric plot:
- **T_{eff} increases continuously with activity f !**

This method is powerful but an implementation in actual experiments is dubious...better use **tracers**

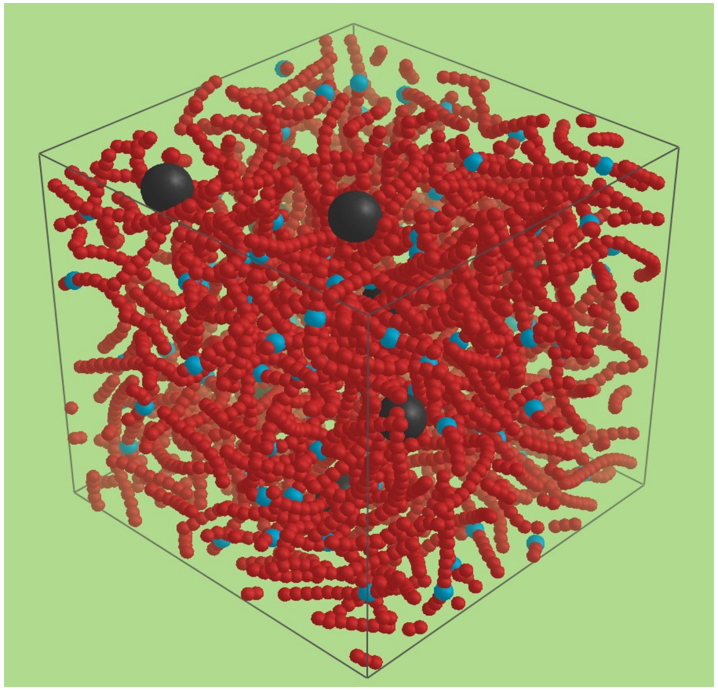
Effective temperatures II: tracers

- A micrometric intruder (**tracer**) is immersed in the active system and **couples to the polymer matrix**
- Its **free** or **driven** dynamics provide information about the polymer melt
- We follow the dynamics of the tracer both **free** and **pulled** by a small force $\mathbf{h=h_x}$
- We determine T_{eff} via the Einstein relation between **diffusion** and **mobility**

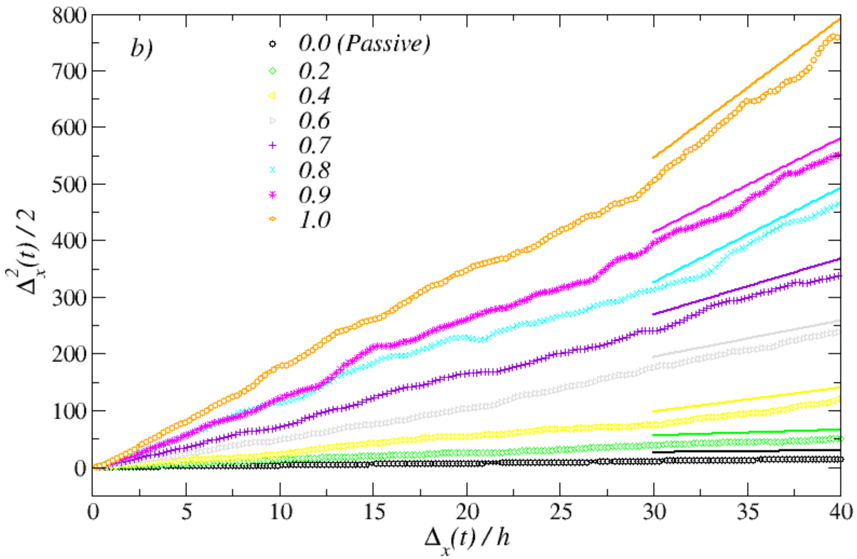
free $$\Delta_x^2(t)=\frac{1}{N_{tr}}\langle\sum_i^{N_{tr}}|x_i^{tr}(t)-x_i^{tr}(0)|^2\rangle$$

driven $$\Delta_x(t)=\frac{1}{N_{tr}}\langle\sum_i^{N_{tr}}|x_i^{tr}(t)-x_i^{tr}(0)|\rangle$$

$$\frac{\Delta_x^2(t)}{2}=T_{eff}\frac{\Delta_x(t)}{h}$$



Effective temperatures III: tracers again

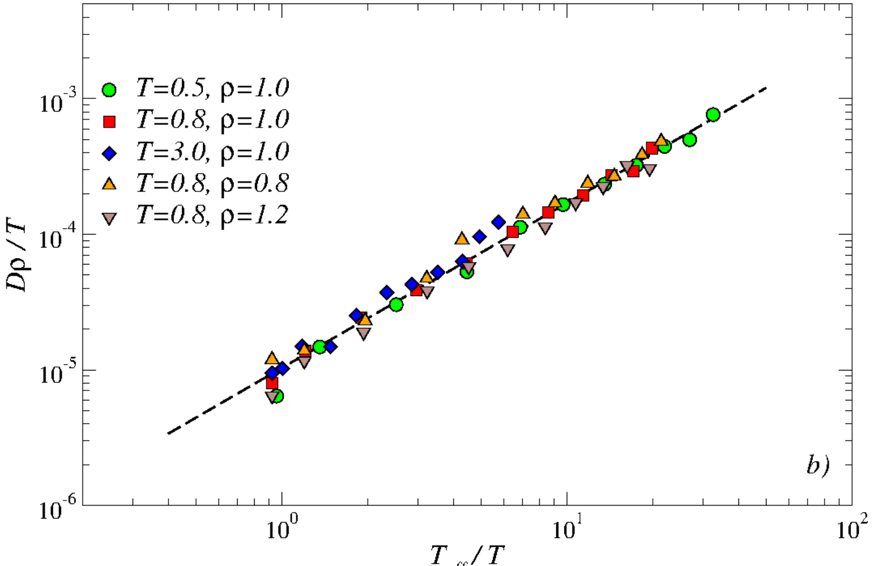


- T_{eff} can be calculated by linear fitting (solid lines)
- Again, T_{eff} is controlled by motor activity
- Use of **massive free** tracers has also been considered

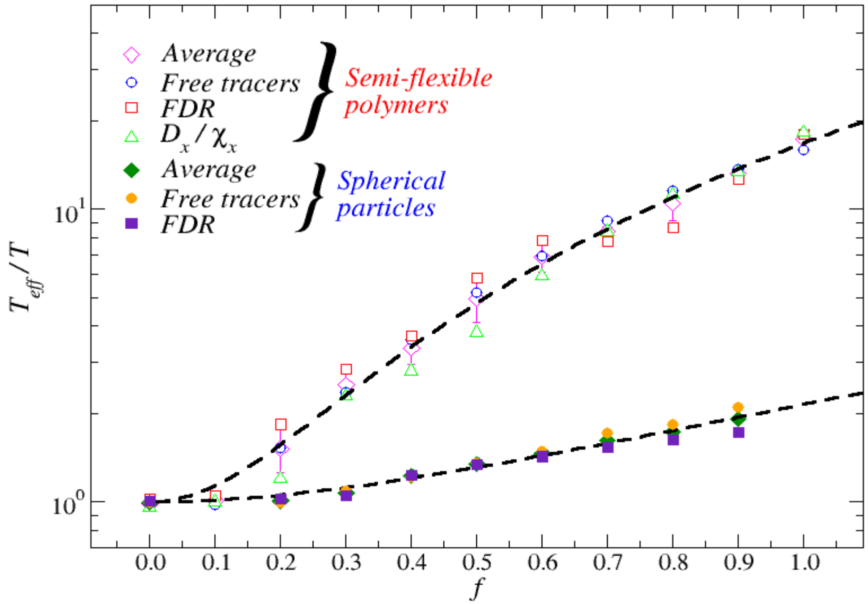
- Consider **different T and ρ** and calculate D and T_{eff}
- All data can be collapsed on a **master curve**

$$D\rho/T \propto (T_{eff}/T)^{\alpha}, \alpha \simeq 1$$

- Once the master curve is known we can **predict** T_{eff} by just computing D of a free tracer...



Effective temperature(s) vs motor activity



$$\frac{T_{eff}}{T} = 1 + \gamma f^2$$

- All available data, both for **self-propelled particles & motorized semi-flexible filaments**
- Different methods used (FDR, massive and driven tracers), all give **consistent results**
- In active systems T_{eff} seems to have a thermodynamic **meaning**
- Different values of T_{eff} correspond to different structure and dynamics
- T_{eff} reflects the motor activity (similar to the Peclet number...)

Conclusions & perspectives

- The out-of-equilibrium steady-state of **active matter** (internal non-conservative stimuli) can be characterized by a simple parameter, the **effective temperature** T_{eff}
- T_{eff} seems to depend continuously on the **motor activity**
- **Different methods** give compatible results for T_{eff}
- **Tracer particles** seems to be very-well suited for T_{eff} measures in **experiments**
- Much to be investigated...

  - We need to develop more realistic motors: from **random** to **selective** motors...
  - Can we observe a $\mathbf{T_{eff} < T}$?
  - What about **mechanical properties** (i.e., elastic constants)?
  - ...

Looking for more information?

Non-conservative forces and effective temperatures in active polymers
D. Loi, SM, and L. F. Cugliandolo
Soft Matter 7, 10193 (2011)

Effective temperature of active complex matter
D. Loi, SM, and L. F. Cugliandolo
Soft Matter 7, 3726 (2011)

Effective temperature of active matter
D. Loi, SM, and L. F. Cugliandolo
Phys. Rev. E 77, 051111 (2008)

http://stefano-mossa.weebly.com

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Thank You!