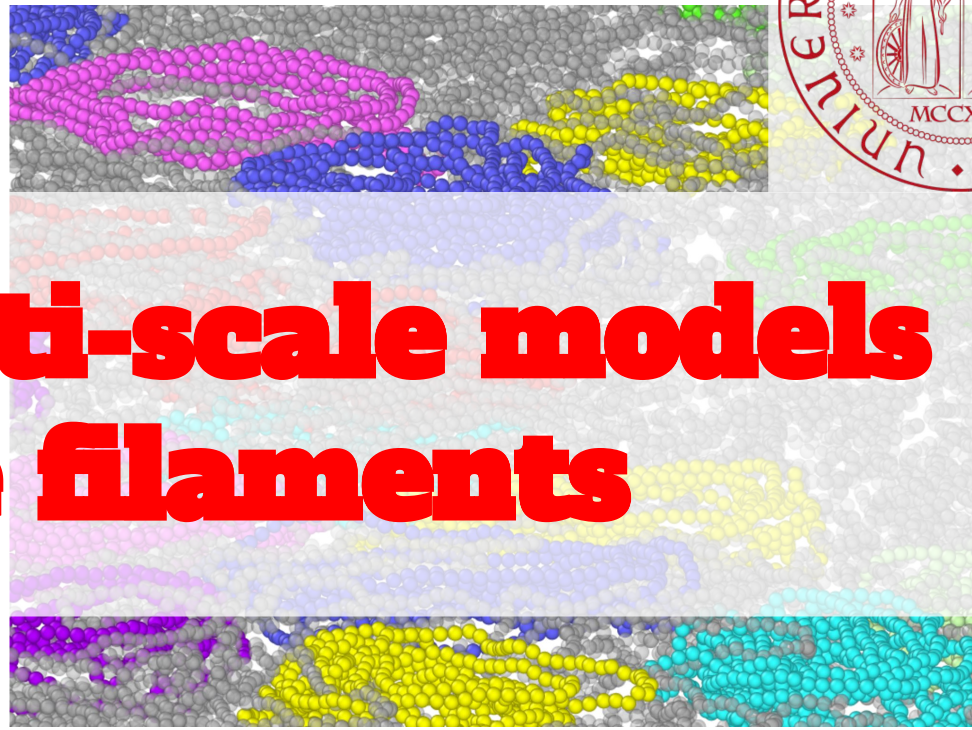
@elocatelli86

http://statphys.dfa.unipd.it/people/locatelli.php



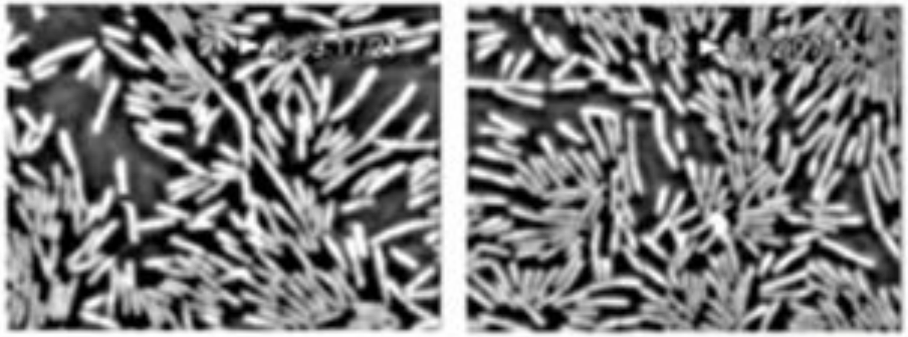
Towards multi-scale models of active filaments

Emanuele Locatelli

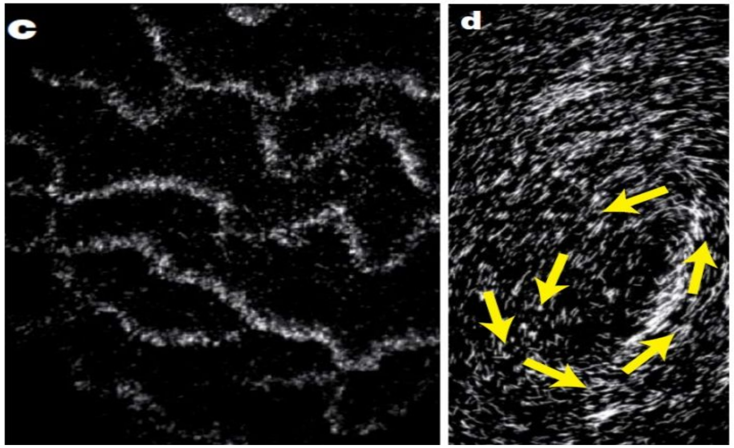
Department of Physics and Astronomy,
University of Padova

ECT* Workshop, Trento, 19-04-2024

Active Matter

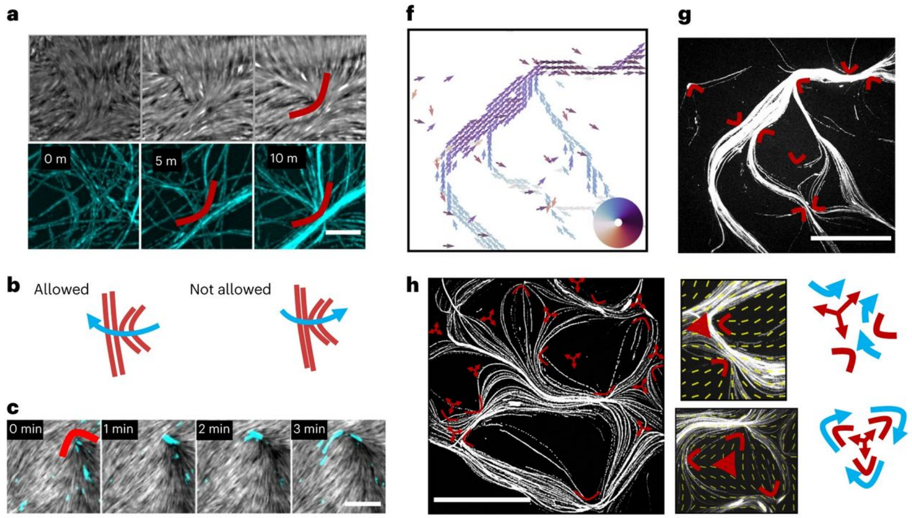


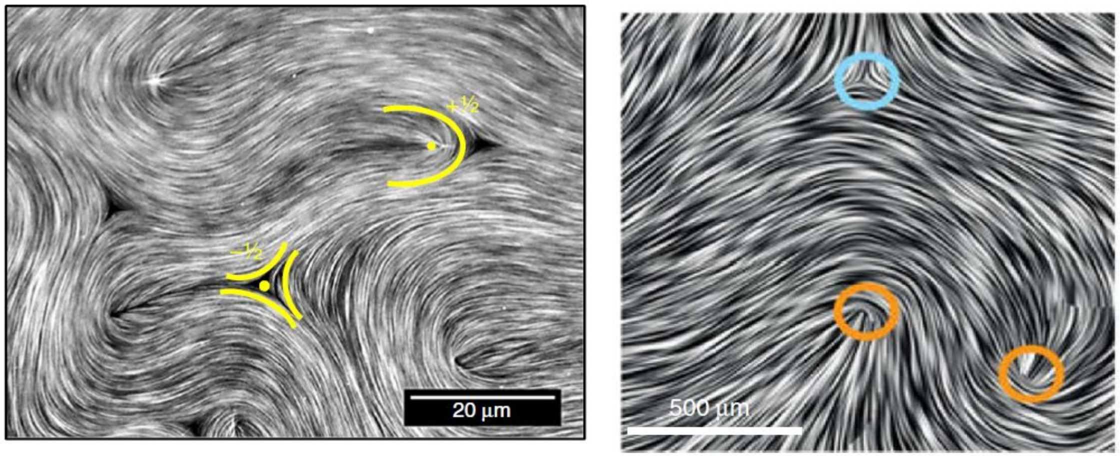
Active Polymeric Matter



Active filaments (Active Nematics)
Nature, 467 (2010).

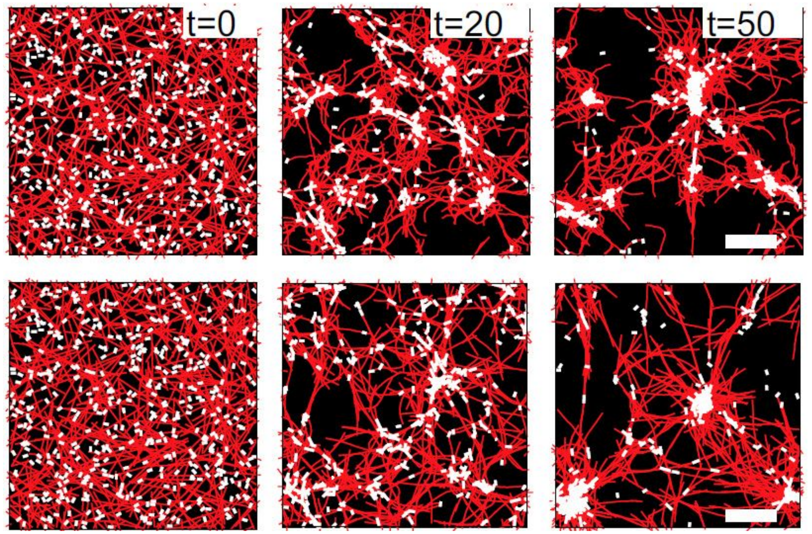
Nature Materials 22, 260–268 (2023)





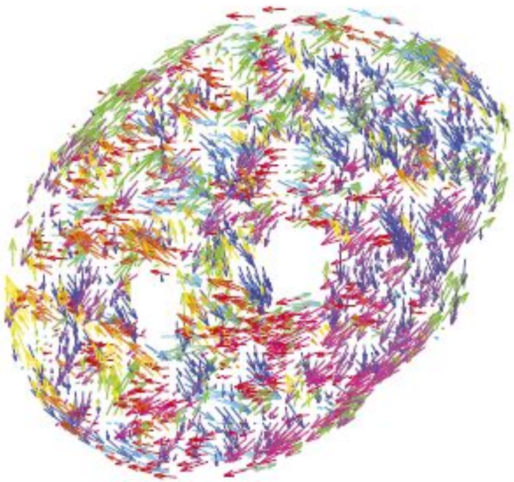
Nat. Comm. 9, 1, 3246 (2018)

Active Polymeric Matter



Active intracellular processes

Nature, 416 (2002)| PNAS, 114 (2017)
Nature Physics 11, 2, 111 (2015).



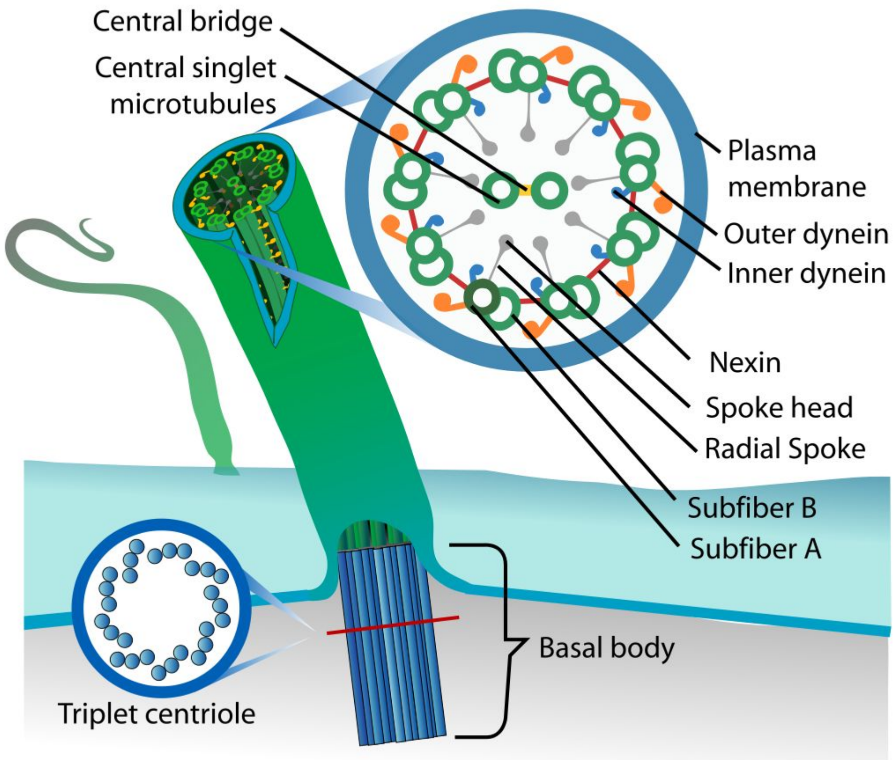
Collective motion interphase chromatin

PNAS 110, 15555–15560 (2013)| PNAS 115, 45, 11442-11447 (2018)| PRX 12, 041033 (2022) | PRL 131, 048401 (2023)

Chromatin organization

PRL 126, 158101 (2021)| Soft Matter,19, 1348-1355 (2023)| Soft Matter, 18, 8134-8146 (2022)| Biophys. J. 106, 9, 1871-1881 (2014)| Phys. Rev. E 99, 032421 (2019) | PNAS 120 e2221726120 (2023)

Active Polymeric Matter



Source: Wikipedia

Cilia carpet in lung cells

Cilia in eukaryotic cells

Science 337: 937-941, (2012)| Annu. Rev. Physiol., 77:379 (2015)| Nat. Phys., 16 1158–1164 (2020)

Modelisation with active polymers

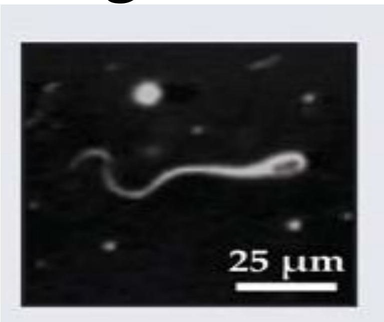
Sci. Rep. 7, 16758 (2017)| Soft Matter,15, 7926 (2019)| J.Chem.Phys 146, 154901 (2017)|Phys. Rev. E 106, 054501 (2022)

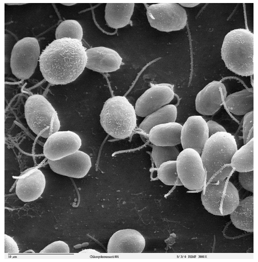
J. R. Soc. Interface 11:20130884 (2013) | J. R. Soc. Interface 14: 20170491 (2017) | Sci. Rep. 3, 1964 (2013) |PRFluids 4, 043102 (2019)|PRL 123, 208101 (2019)

Active Polymeric Matter

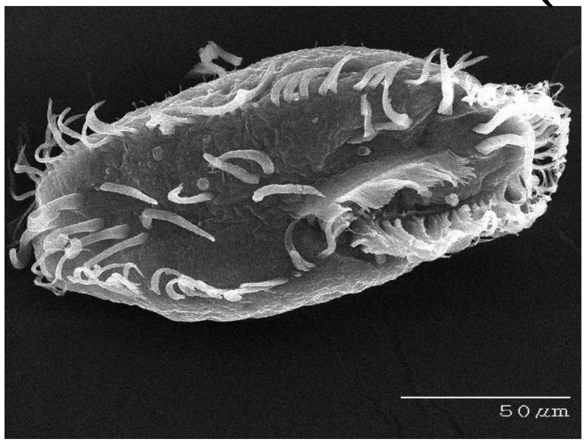
Microswimmer locomotion

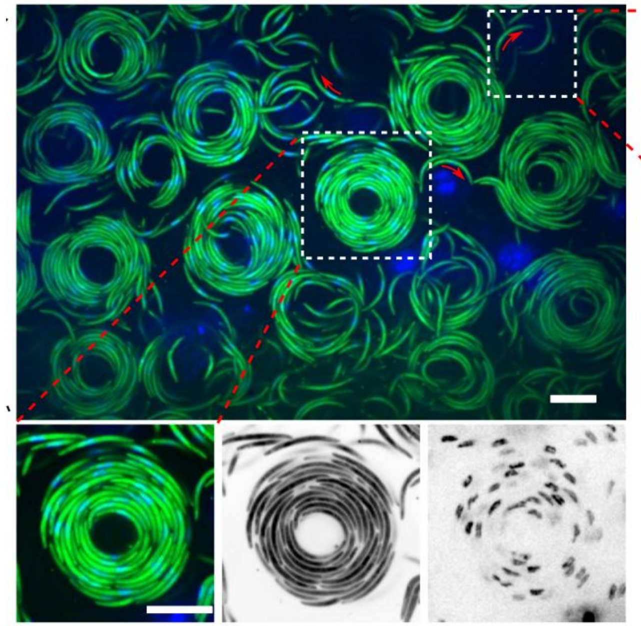
Flagella locomotion (Spermatozoa, C. Reinhardtii)





Cilia locomotion (Ciliate)





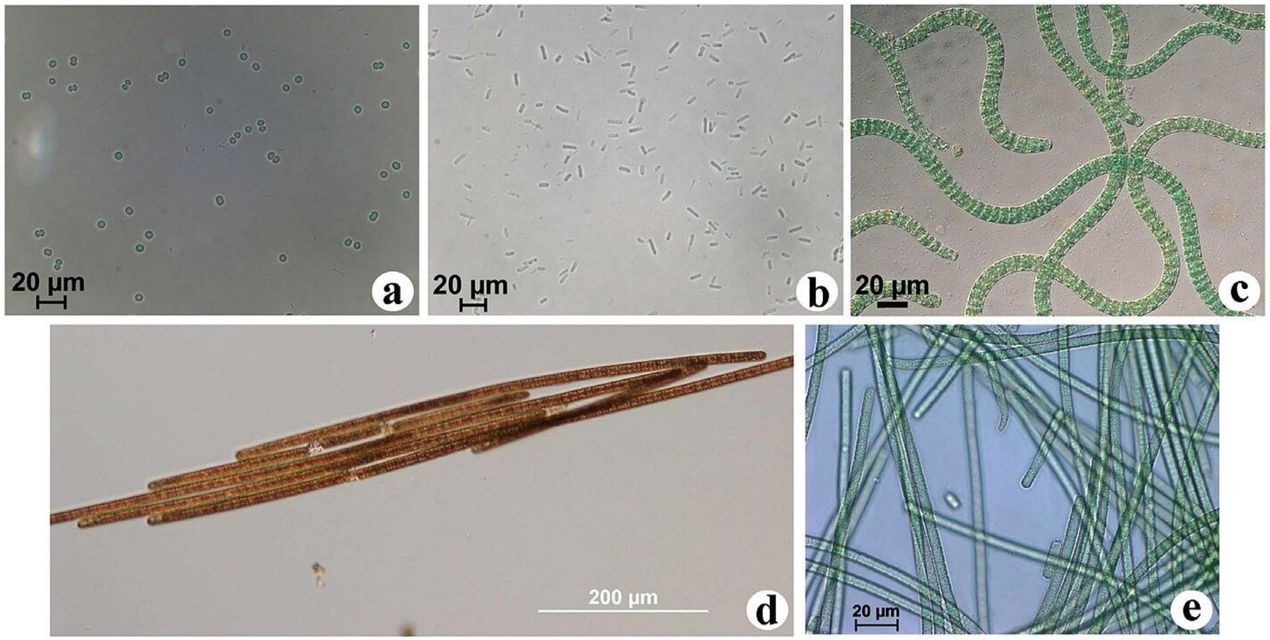
Plasmodium sporozites,
Nat. Phys. 18, 586-594 (2022)

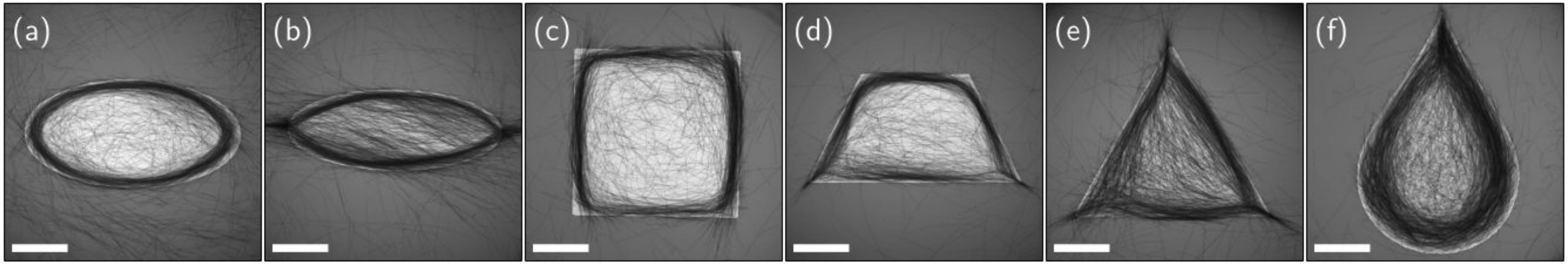
Active Polymeric Matter

Microswimmer locomotion

Cyanobacteria

Scientific American 270.1 (1994): 78-86.
eLife 12 (2023)
Mol. Microbiol. 98, 1021 (2015)
arXiv:2403.03093





Active Polymeric Matter

Macroswimmers: *Tubifex Tubifex* & other worms

Organization
Nat. Comm. 10.683 (2019)| arXiv:2301.11667 (2023)

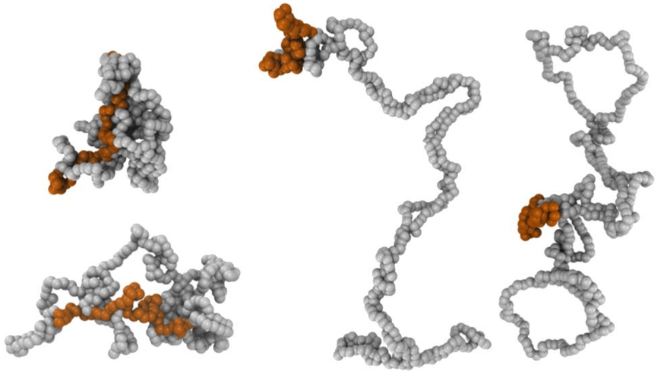
Dynamics & Rheology
Soft Matter, 18, 1174 (2022)| Nat. Phys., 17, 275-283 (2021)| PNAS 116, 51, 25569–25574 (2019)| arXiv:2303.00647| PRL 124, 188002 (2020)| Sci. Adv., 8, eabj7918 (2022)

Phase separation
PRL 124, 208006 (2020)| PNAS, 118, 2010542 (2021)| Front. Phys., 9, 734499 (2021)

Entanglement & collective motion
Int. & Comp. Biol., 62, 890-896 (2022)| Science 380.6643 (2023)| Soft Matter 19,10 (2023)

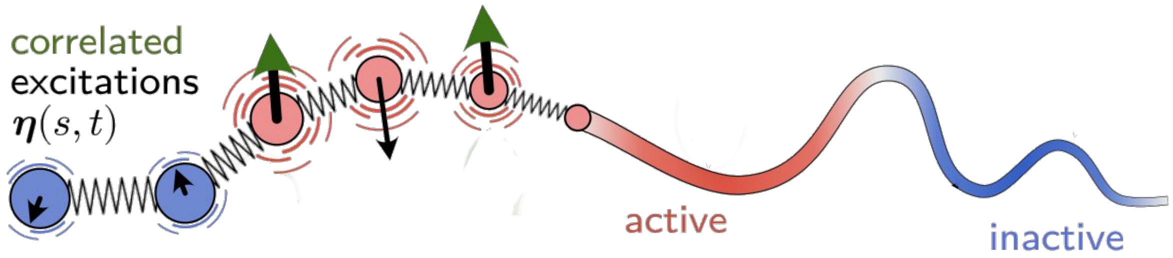
Active Polymer Models

2-temperature model



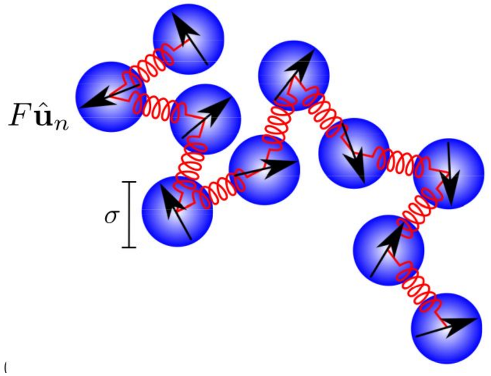
From: Nat. Comm. 11, 26 (2020)

Correlated noise



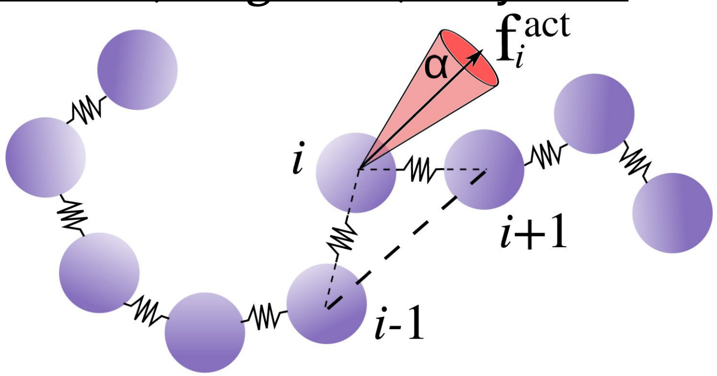
From: PNAS 120 e2221726120 (2023)

Active Brownian Polymers



From: J.Chem.Phys. 142, 124905 (2015)

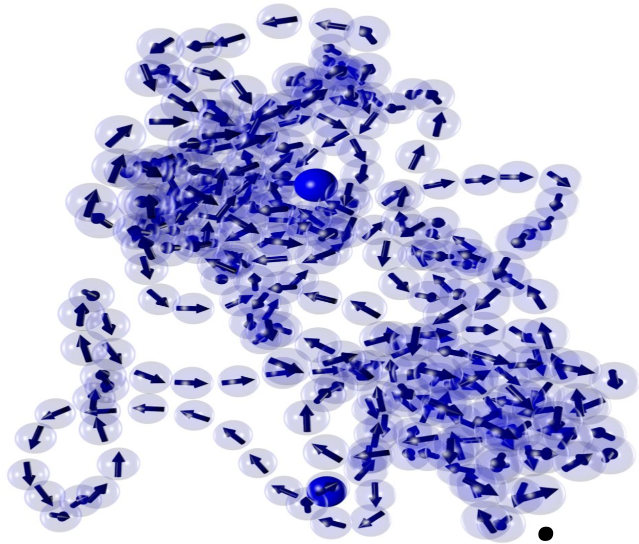
Active Polar (Tangential) Polymers



From: PRL 121, 217802 (2018)

Outline

Polar Active Polymers

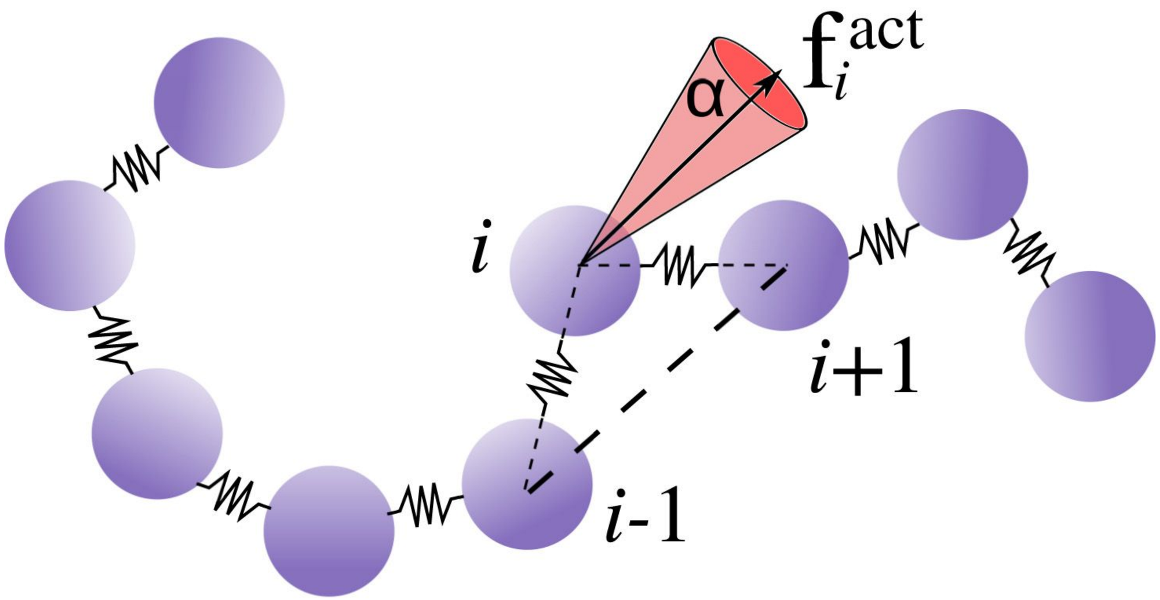


Multi-scale analysis of dense suspensions

Towards modeling biophysical systems

Polar Active Polymer

Polar (tangential) self-propulsion



Decorrelation/relaxation time

$$\tau \frac{D_0}{\sigma^2} \sim \frac{N}{Pe}$$

Total active force

$$\mathbf{F}^{\mathrm{act}} = \sum_i^N \mathbf{f}_i^{\mathrm{act}} \approx \mathbf{R}_E$$

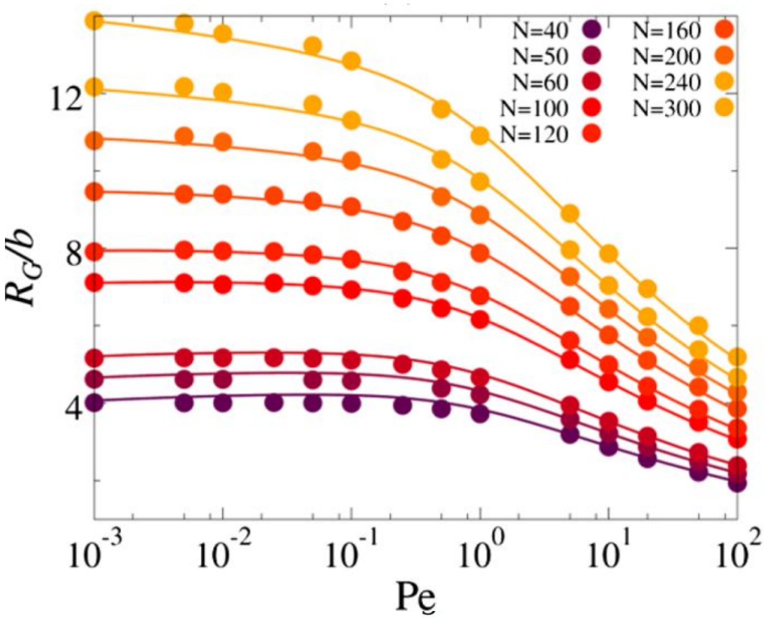
$$\mathrm{Pe} \equiv \frac{v^{\mathrm{act}} b}{D_0} = \frac{f^{\mathrm{act}} b}{k_B T}$$

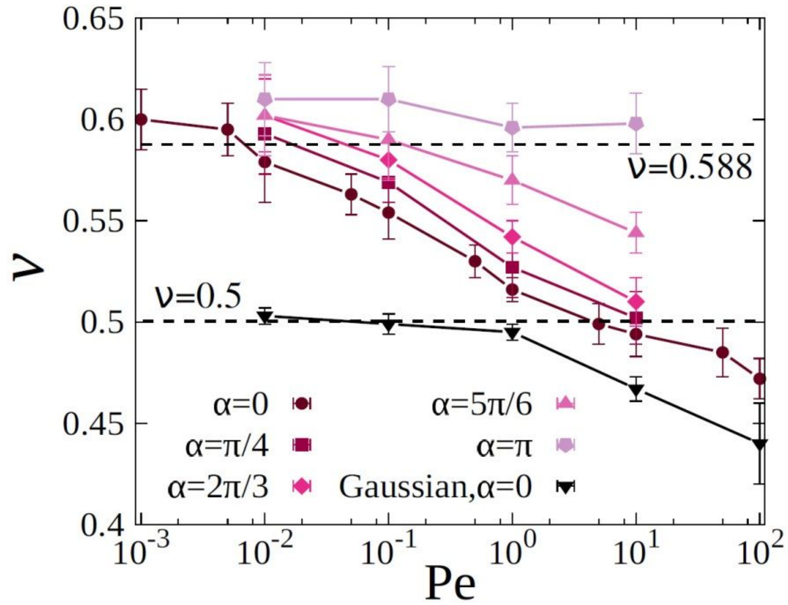
V. Bianco, E. Locatelli, P. Malgaretti, PRL, 121, 217802 (2018)

Polar Active Polymer

Radius of gyration $R_g^2 = \frac{1}{N}\sum_i (\mathbf{r}_i - \mathbf{r}_{cm})^2$

Scaling exponent $< R_g > \propto N^\nu$





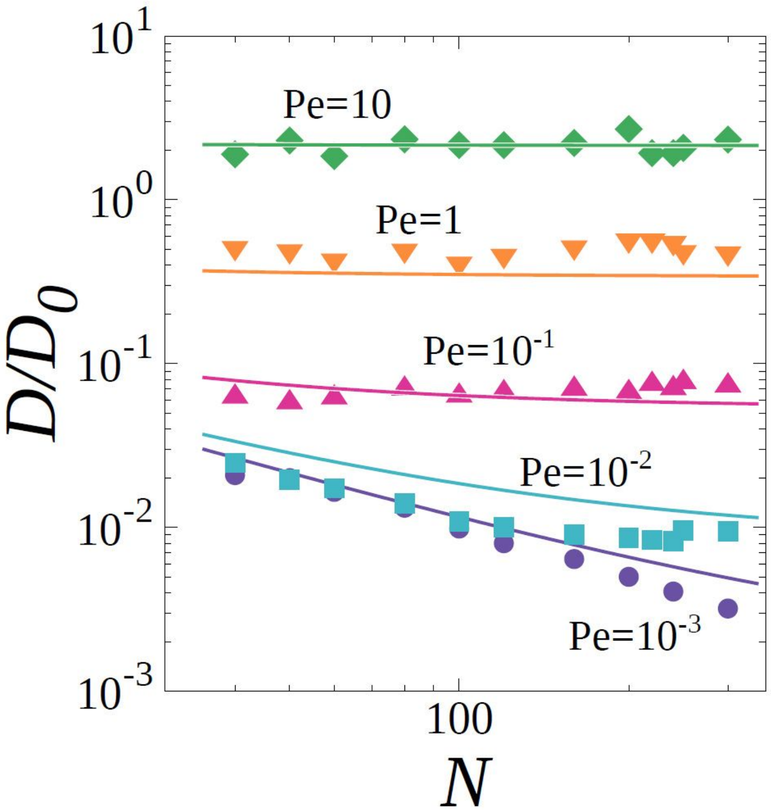
Coil-to-globule-like transition: the polymer becomes more compact (bundled) for higher values of Pe

Due to follower-forces instability (akin to buckling instability)

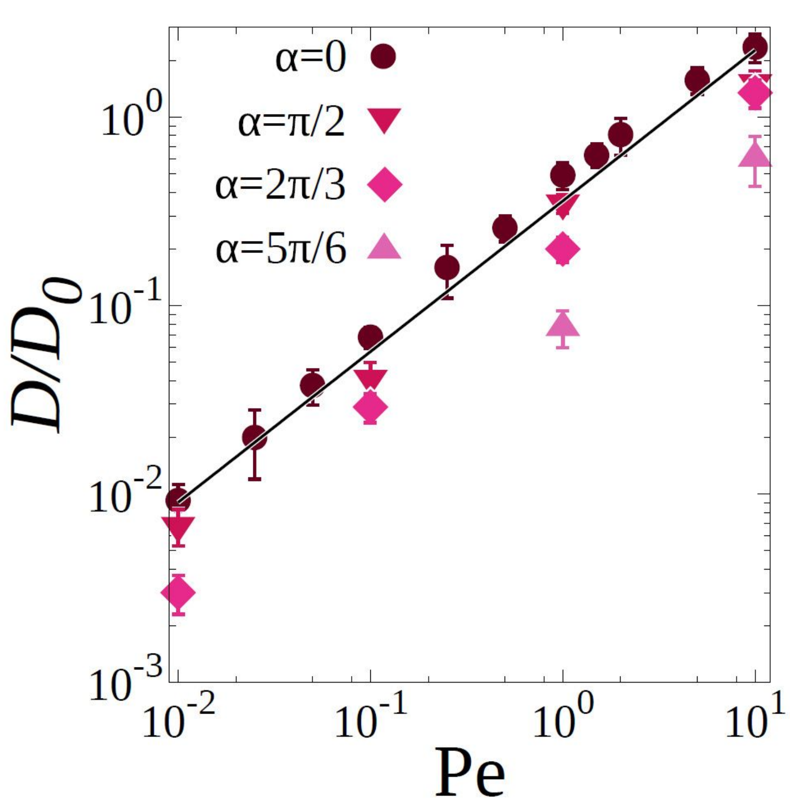
V. Bianco, E. Locatelli, P. Malgaretti, PRL, 121, 217802 (2018)

Polar Active Polymer

$$D \propto N^0$$



$$D \propto \mathrm{Pe}^{0.8-0.9}$$



V. Bianco, E. Locatelli, P. Malgaretti, PRL, 121, 217802 (2018)

Polar Active Polymer

Minimal stochastic model for the dynamics of the center of mass

$$\dot{\mathbf{r}}_{CM} \equiv \frac{1}{N}\sum_{i}^{N} \dot{\mathbf{r}}_i = \frac{1}{N}\left(\boldsymbol{\xi} + \boldsymbol{\eta}\right)$$

$$\boldsymbol{\xi} \equiv \frac{1}{\zeta}\mathbf{F}^{\mathrm{act}} = \frac{1}{\zeta}\sum_i^N \mathbf{f}_i^{\mathrm{act}}$$

$$\boldsymbol{\eta} \equiv \frac{1}{\zeta}\sum_i^N \boldsymbol{\eta}_i$$

As $\mathbf{F}^{\mathrm{act}}$ is almost parallel to the end-to-end vector, we model it as a random force with the same decorrelation properties as **C(t)**

$$\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t')\rangle \propto C(t) \equiv \langle \mathbf{r}_E(t)\cdot\mathbf{r}_E(0)\rangle$$

$$D = 2aN^{2\nu(\mathrm{Pe})-1} + \frac{D_0}{N}$$

V. Bianco, E. Locatelli, P. Malgaretti, PRL, 121, 217802 (2018)

Polar Active Polymer

Even simpler approach:

$$D = D_t + \frac{\tau_r \, v_a^2}{2d} = D_t + \frac{\tau_r \, (f_a/\gamma)^2}{2d}$$

Active Brownian Particle

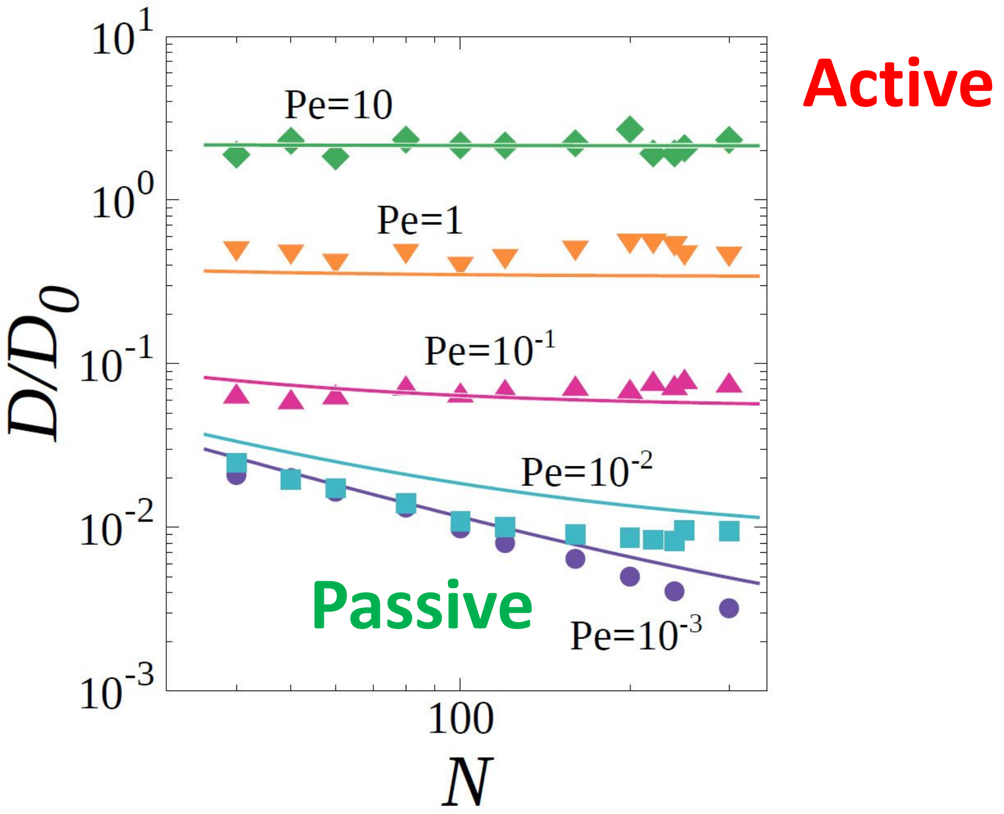
$$\frac{D_a - D_t^P}{D_t^P} = \frac{\tau_r^P D_t}{\sigma^2} \frac{R_e^2}{2N\sigma^2} \mathrm{Pe}^2$$

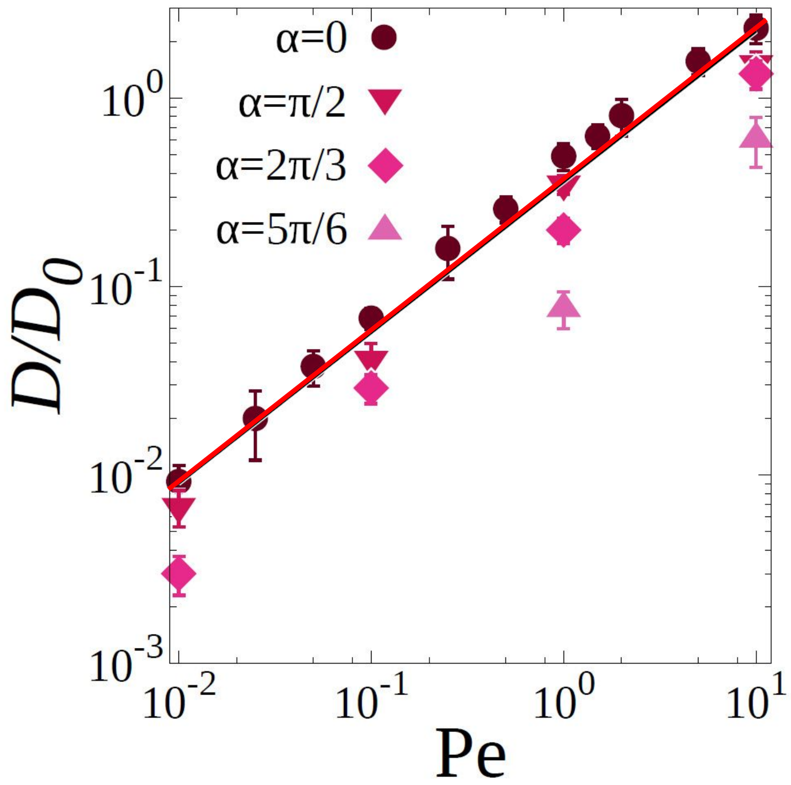
$$\tau_r^P \propto \frac{N}{\mathrm{Pe}}$$

M. Fazelzadeh et al, Phys. Rev. E 108, 024606 (2023); J. Martin-Roca, et al, in preparation

Polar Active Polymer

$$D = \boxed{2aN^{2\nu(\mathrm{Pe})-1}} + \boxed{\frac{D_0}{N}}$$

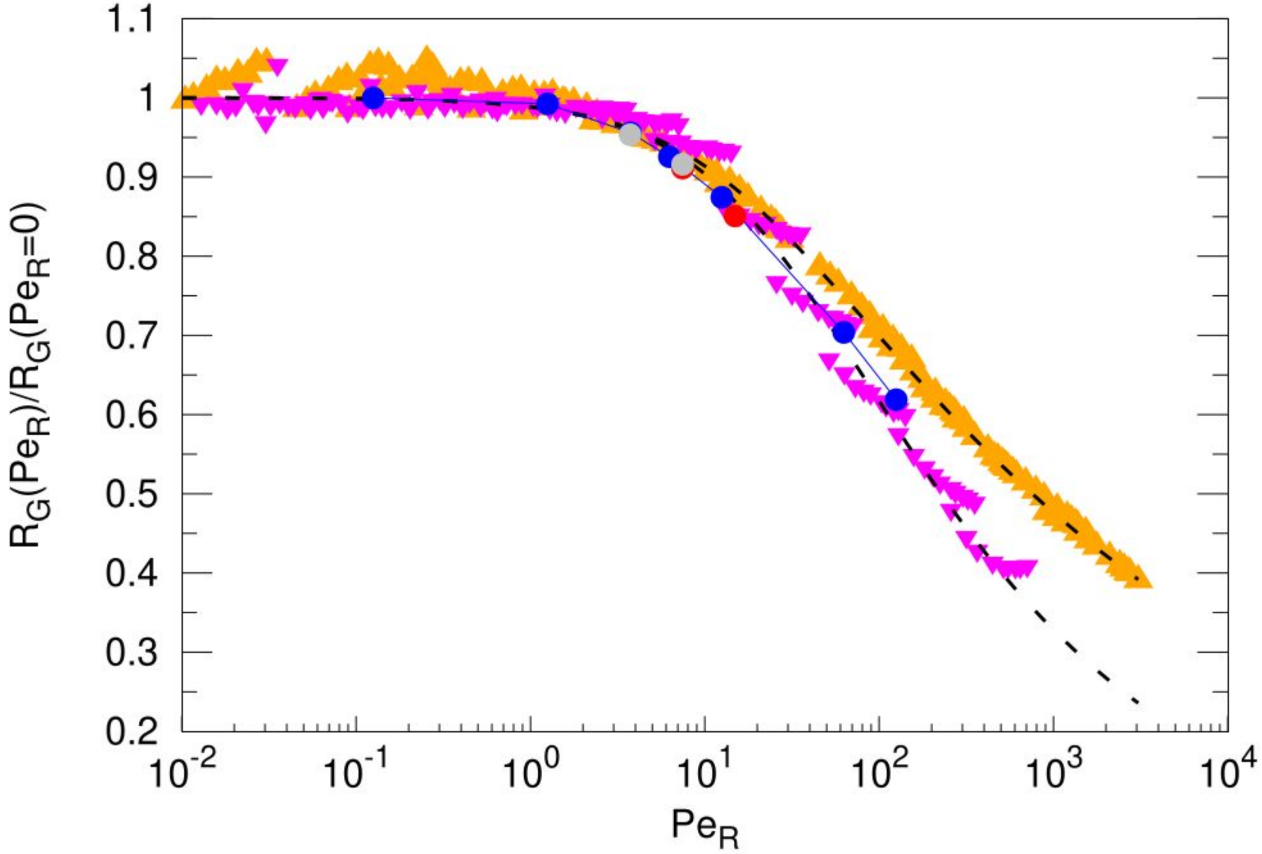




V. Bianco, E. Locatelli, P. Malgaretti, PRL, 121, 217802 (2018)

Polar Active Polymer

Active Rouse Model (with semi-flexibility)

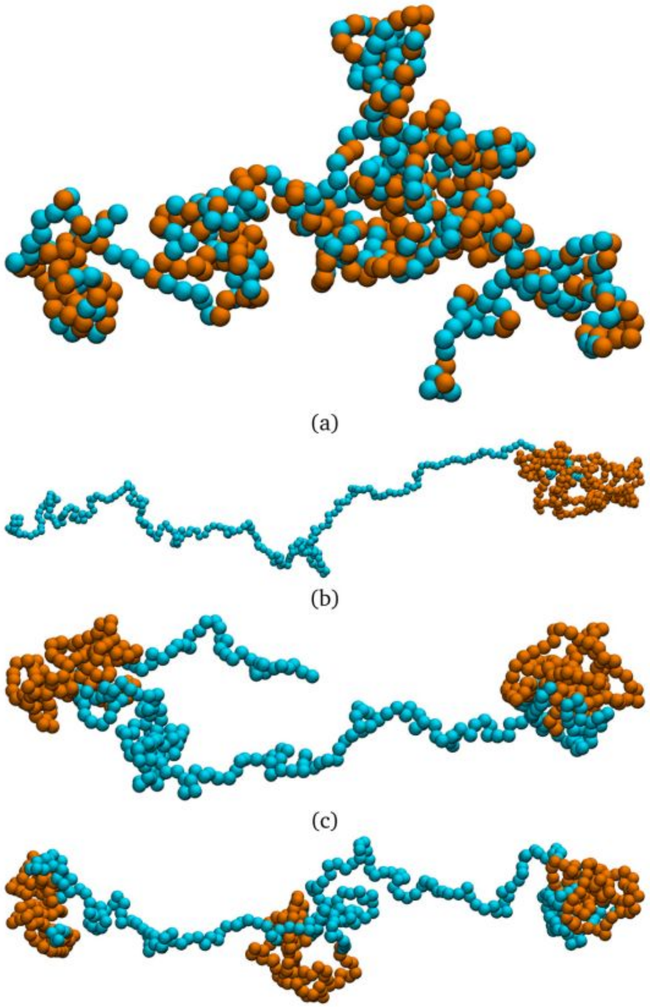


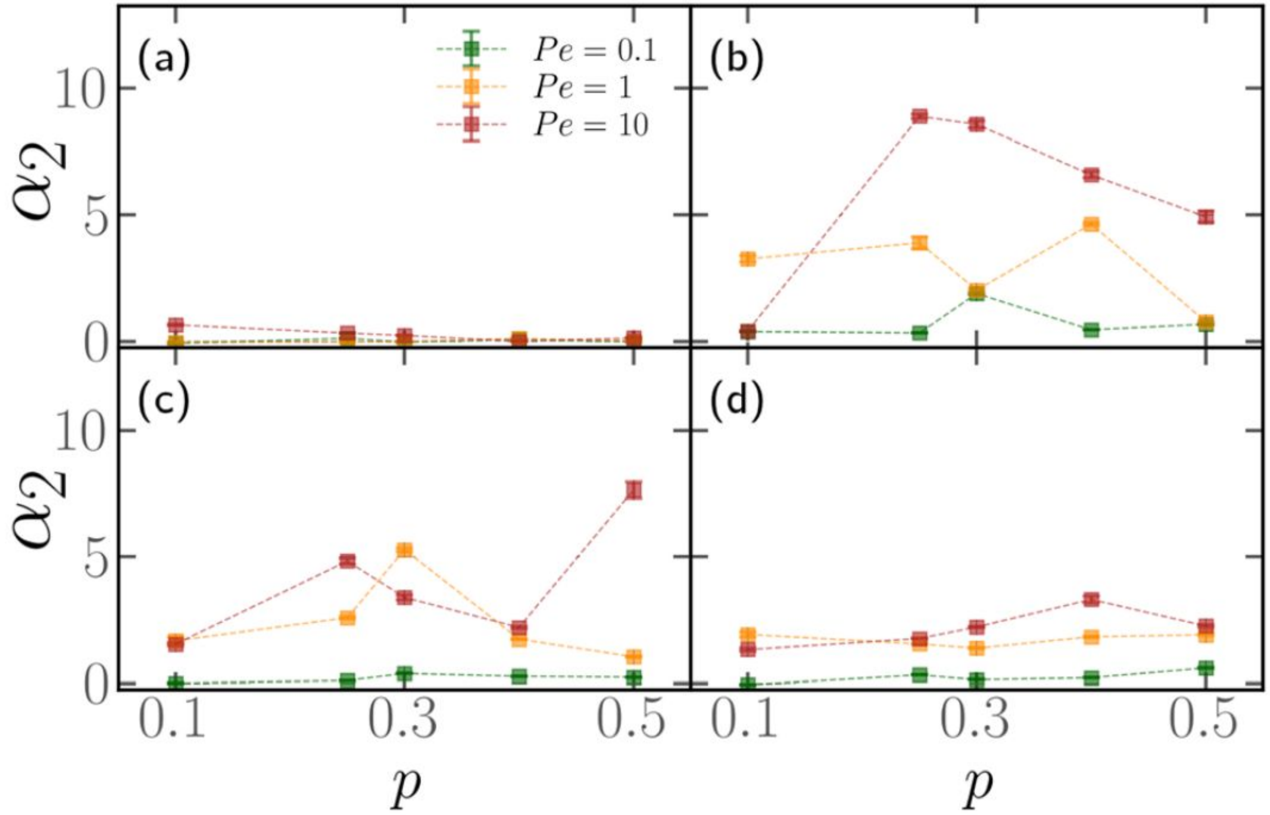
R_g is the relevant length scale of the system

Pe_R=Pe R_g(N,Pe=0)

P. Malgaretti, E. Locatelli, C. Valeriani (submitted)

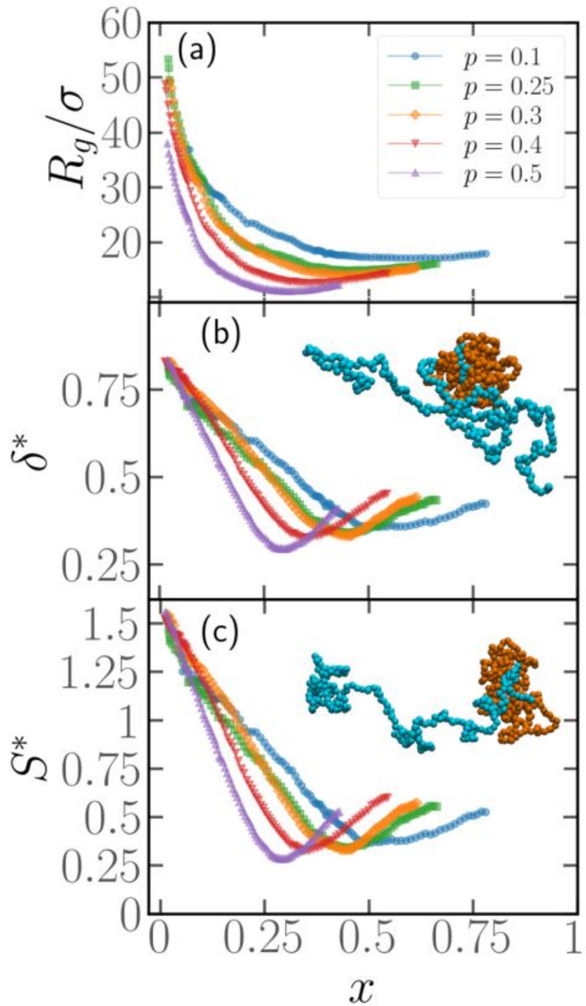
Active Diblock Copolymer

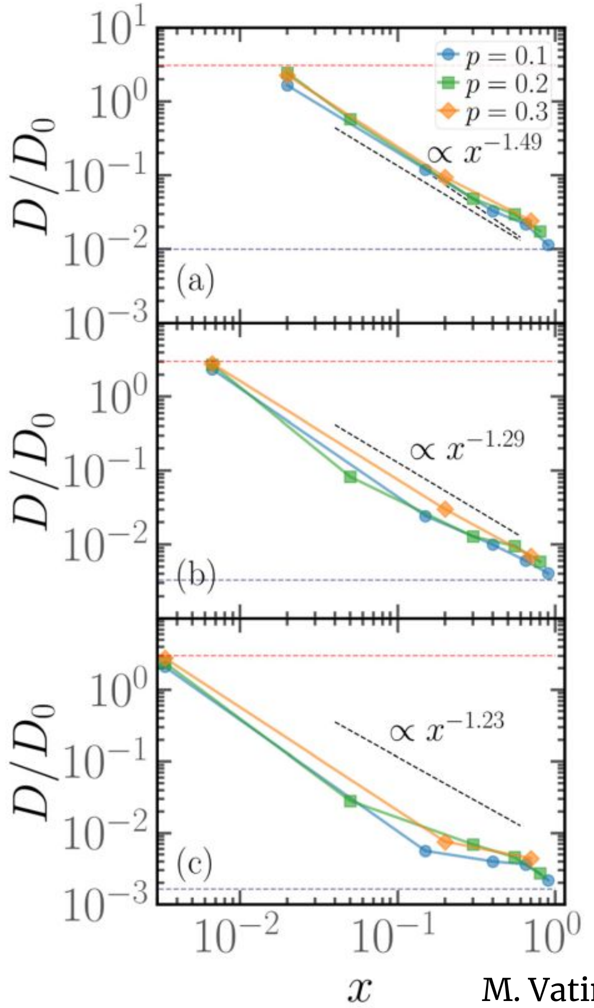


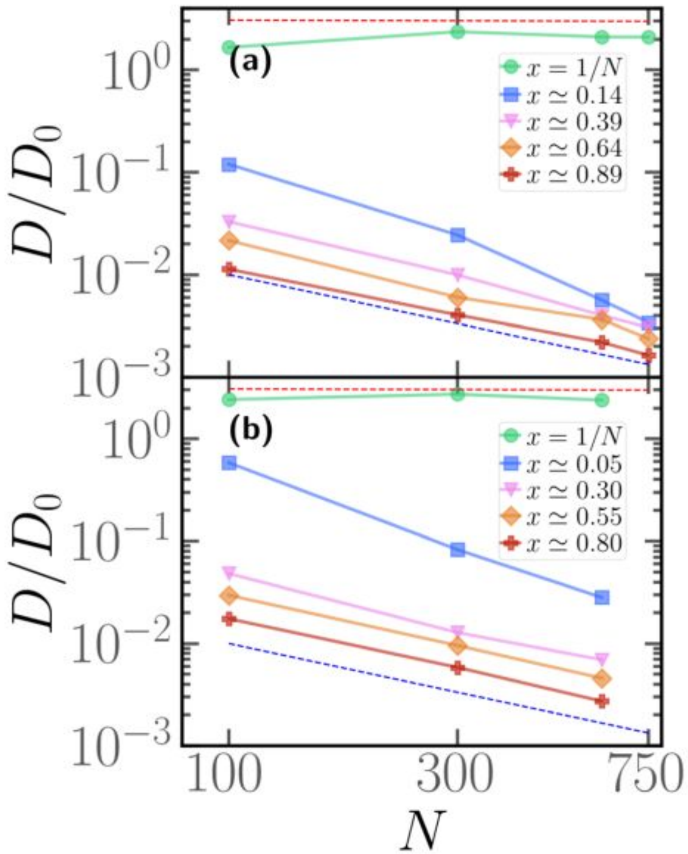


M. Vatin, S. Kundu, E. Locatelli, Soft Matter, 20, 1892-1904 (2024)

Active Diblock Copolymer





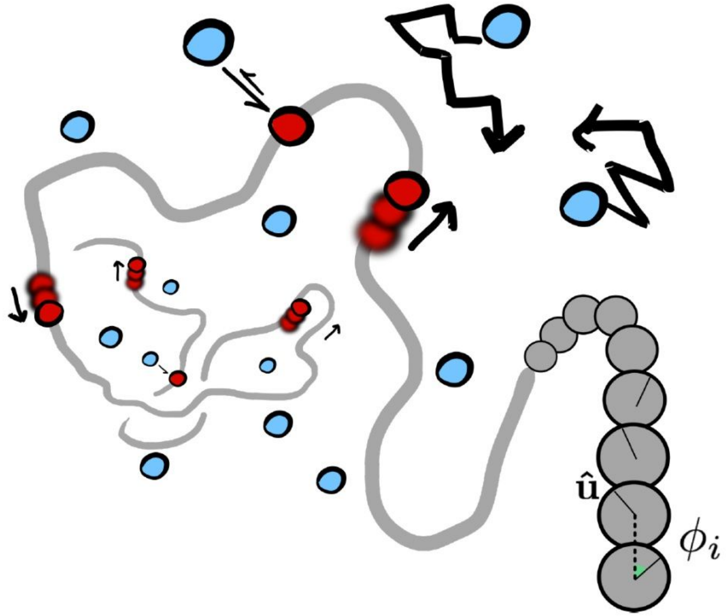


M. Vatin, S. Kundu, E. Locatelli, Soft Matter, 20, 1892-1904 (2024)

Motor-powered Polymer

Semi-flexible polymer substrate of length L

N Freely diffusing motors of size $\boldsymbol{\sigma}$

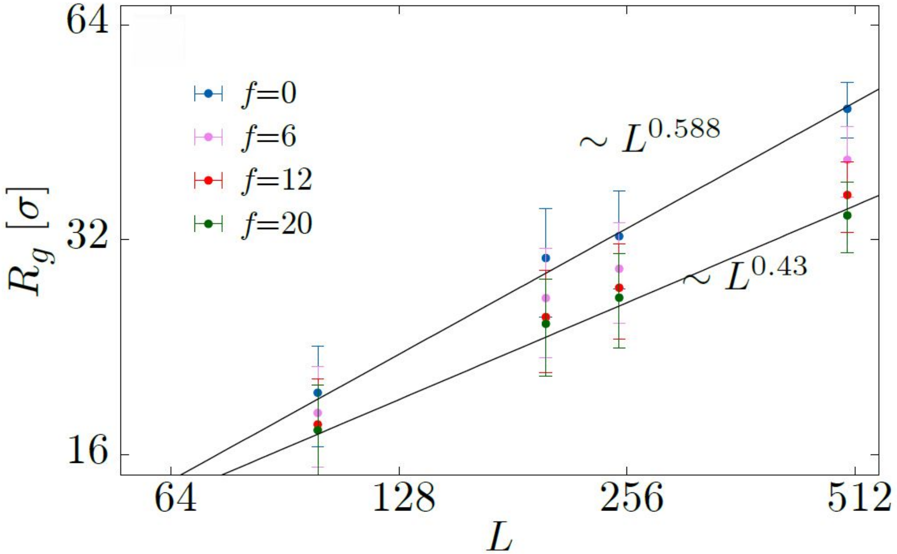


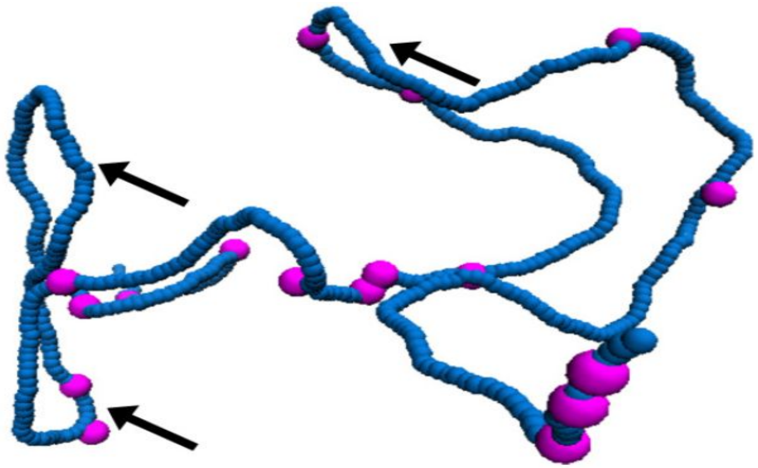
- Average number of bound motors $\langle n \rangle$
- Motor force f
- Binding energy $\boldsymbol{K_{MOT}}$
- Substrate rigidity $\boldsymbol{K}_{\mathbf{BEND}}$

Freely diffusing motors bind to the substrate and propel themselves in the direction of the local bond vector, pushing the polymer in the opposite direction

M. Foglino, et.al, *Soft Matter*, 2019

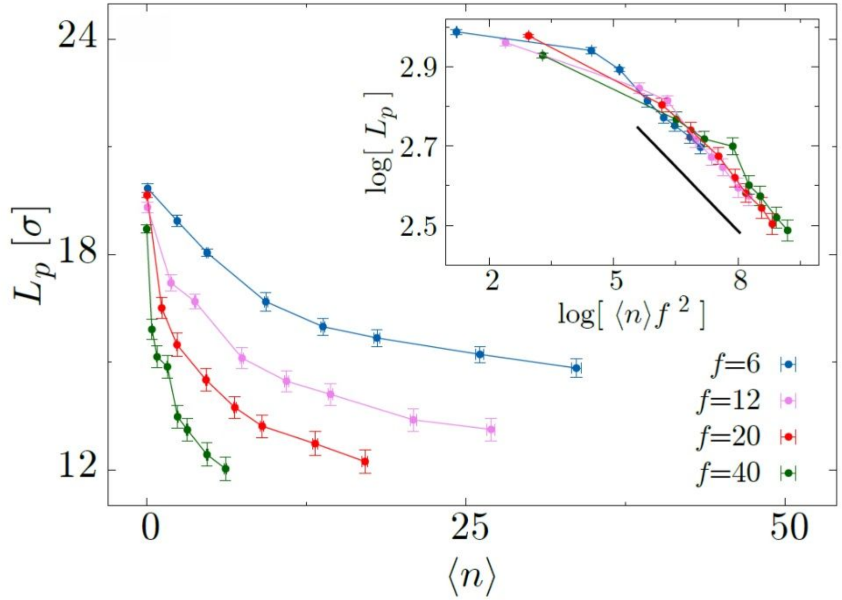
Motor-powered Polymer





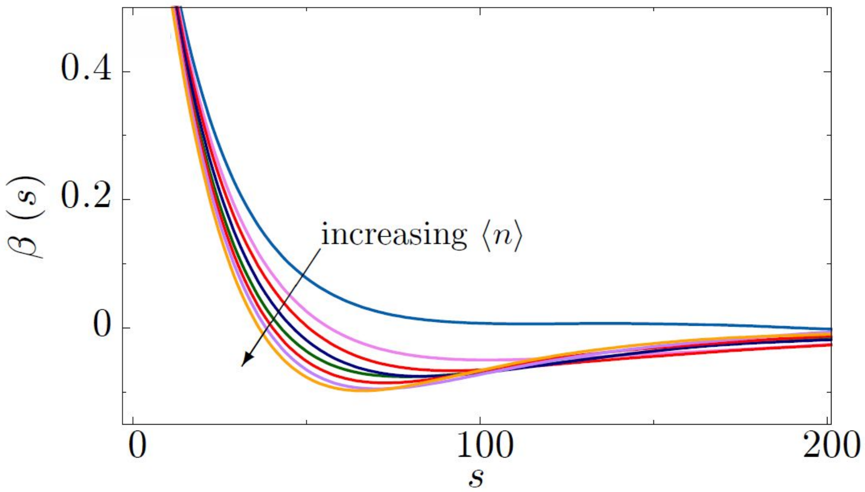
The scaling exponent decreases here too

The buckling instability manifests by the formation of U-shaped tight turns (hairpins) and the “softening” of the substrate



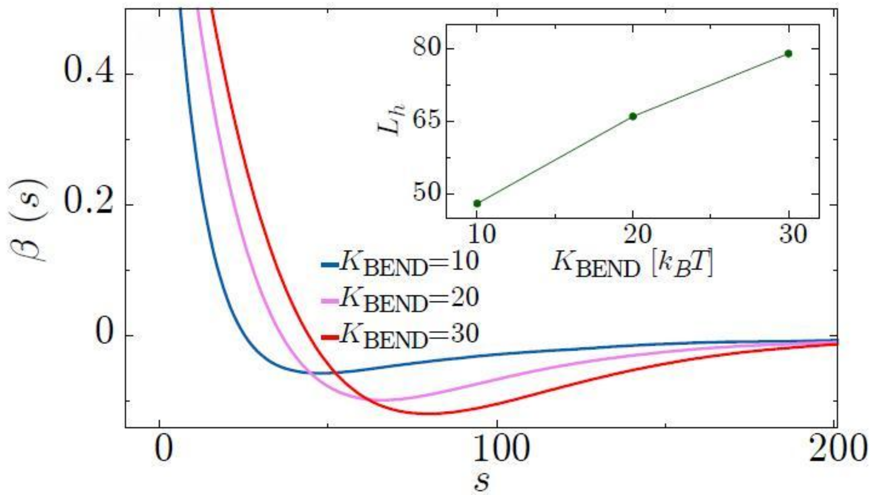
M. Foglino, et.al, *Soft Matter*, 2019

Motor-powered Polymer



$$\beta(s) = \langle \mathbf{b}_i \mathbf{b}_{i+s} \rangle$$

bond autocorrelation function



The bending instability manifests here by the formation of U-shaped rather tight turns (hairpins)

M. Foglino, et.al, *Soft Matter*, 2019

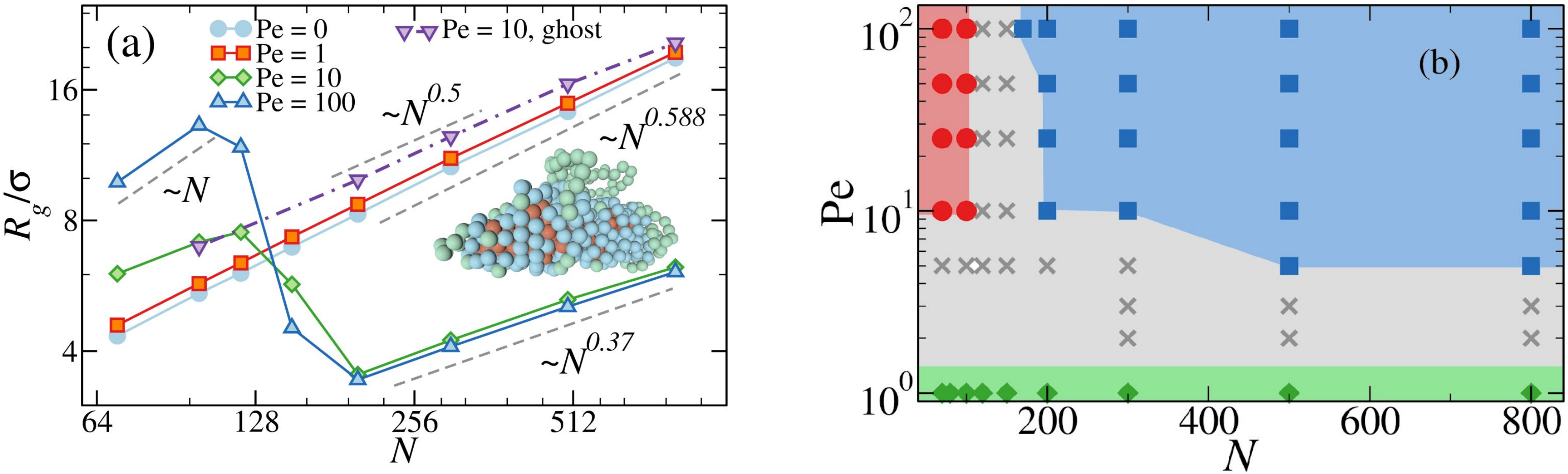
Ring Polymers

Why rings?

- Bacterial DNA is ring shaped; other unicellular parasites organize their DNA into a network of interlocked rings (kDNA)
- Ring polymers (solutions and melts) show distinctive properties, very different from their linear counterpart, despite there is a difference of a single bond
- The effects of circularization are of topological origin (topological repulsion)
- Chromosomes can be modeled as ring polymers

Nature Chemistry 12.5, 433-444 (2020)

Active Ring Polymers



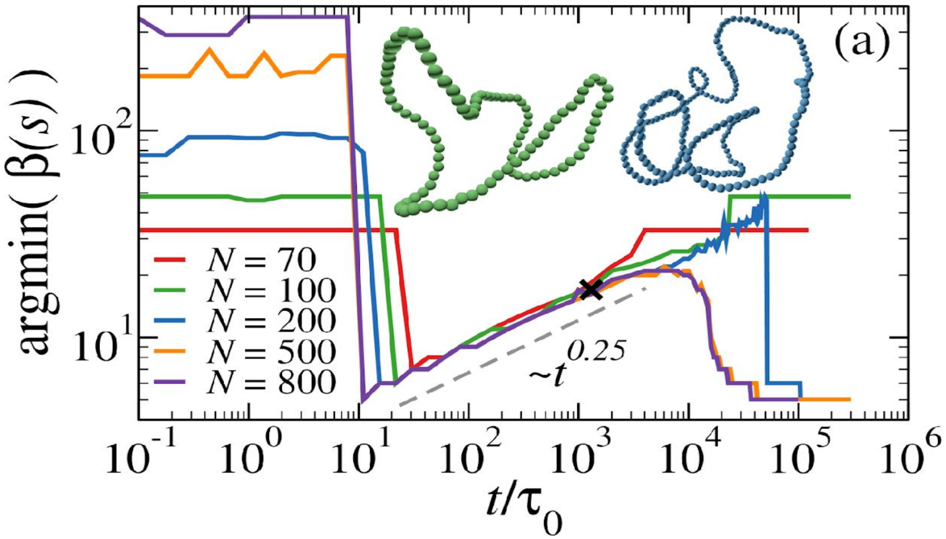
Swelling – collapse transition that becomes sharper at increasing Pe

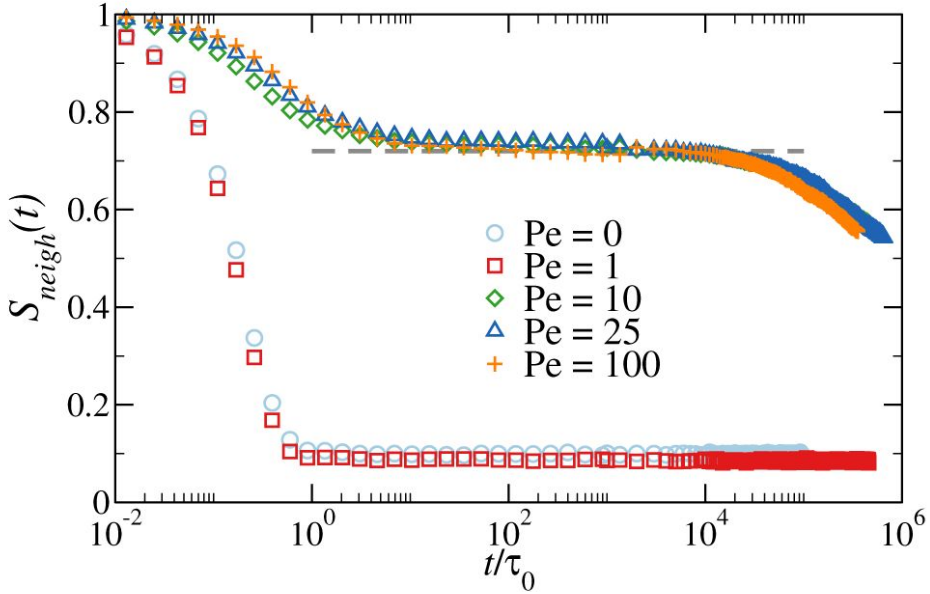
E. Locatelli, V. Bianco , P. Malgaretti, PRL, 126, 097801 (2021)

Active Ring Polymers

Kinetics

Dynamics





Non-equilibrium route from passive conformation to steady state is independent of N

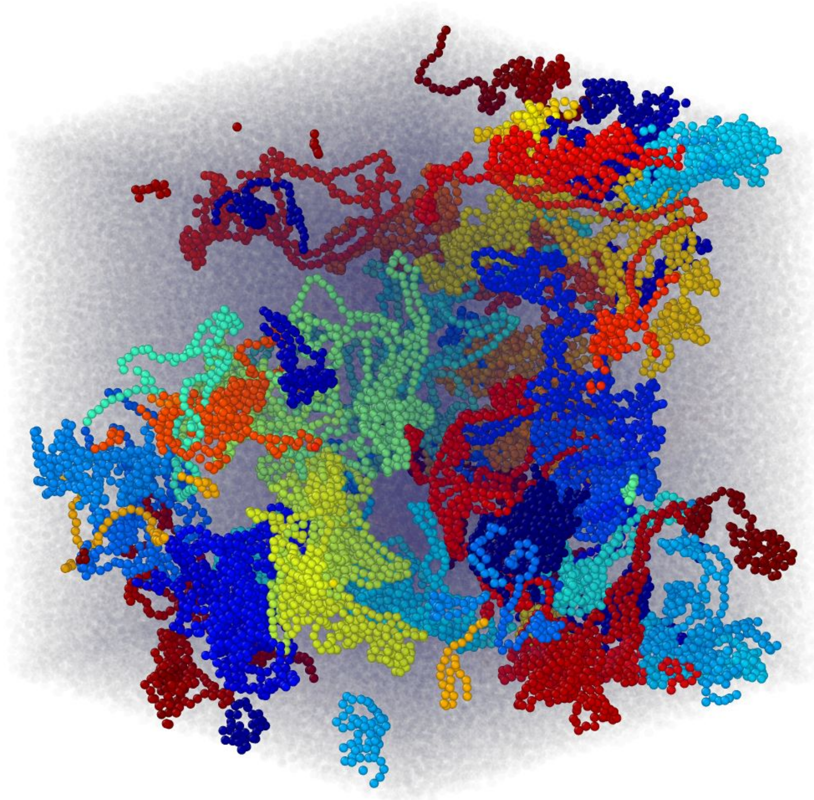
In the steady state, collapsed rings show signs of dynamical arrest in many observables

E. Locatelli, V. Bianco , P. Malgaretti, PRL, 126, 097801 (2021)

Outline

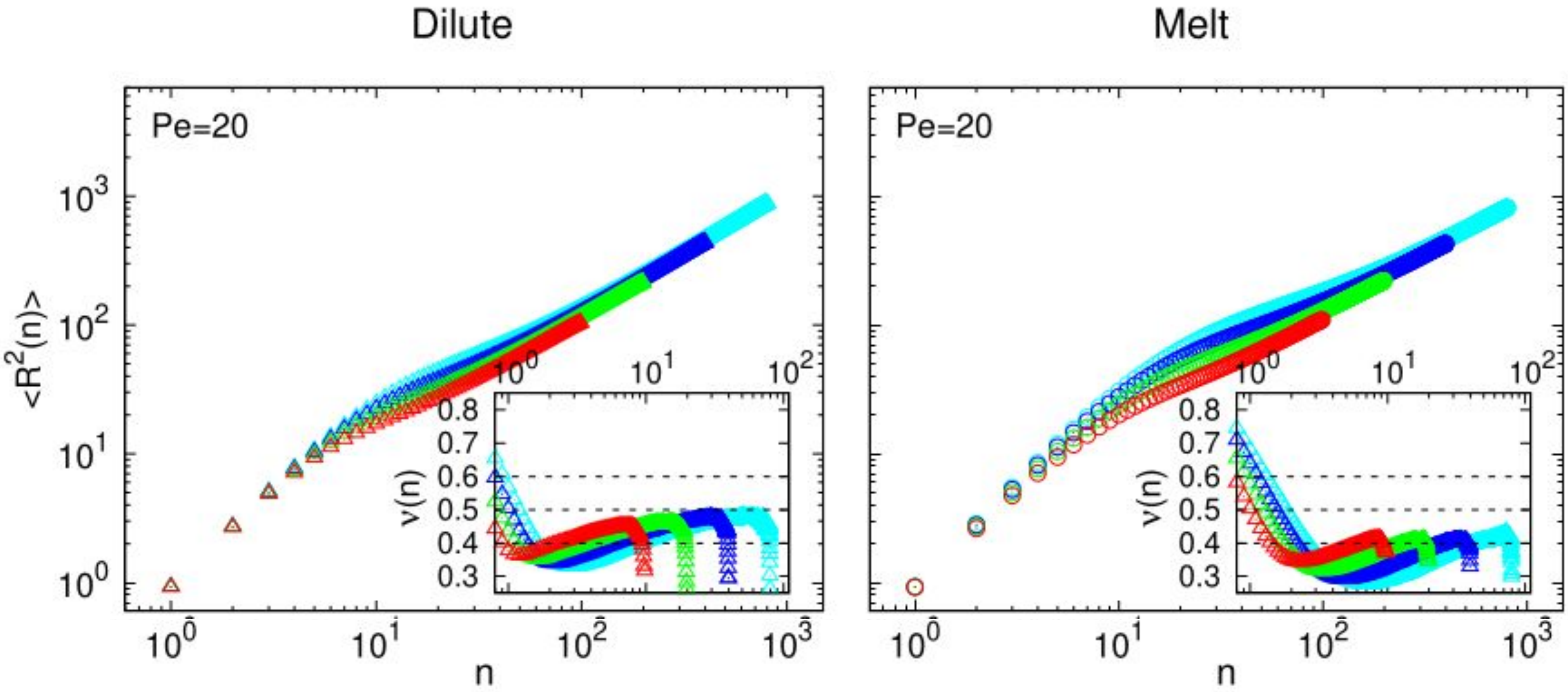
Polar Active Polymers

Multi-scale analysis of dense suspensions



Towards modeling biophysical systems

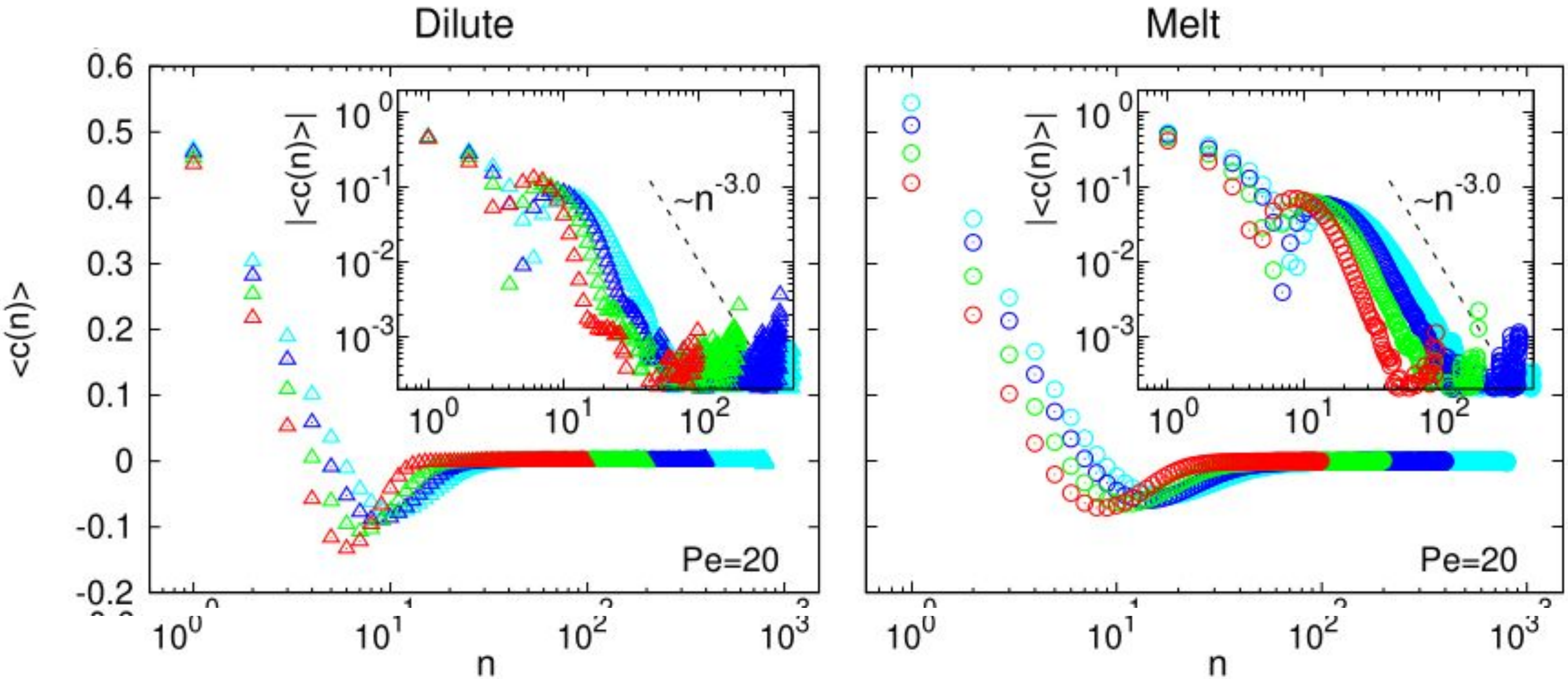
Melts of Active Linear Chains



$$\nu(n) \equiv \frac{1}{2} \frac{\log(\langle R^2(n+1)\rangle) - \log(\langle R^2(n-1)\rangle)}{\log(n+1) - \log(n-1)}.$$

M.A. Ubertini, E.Locatelli, A. Rosa, arXiv:2404.08425 (submitted)

Melts of Active Linear Chains

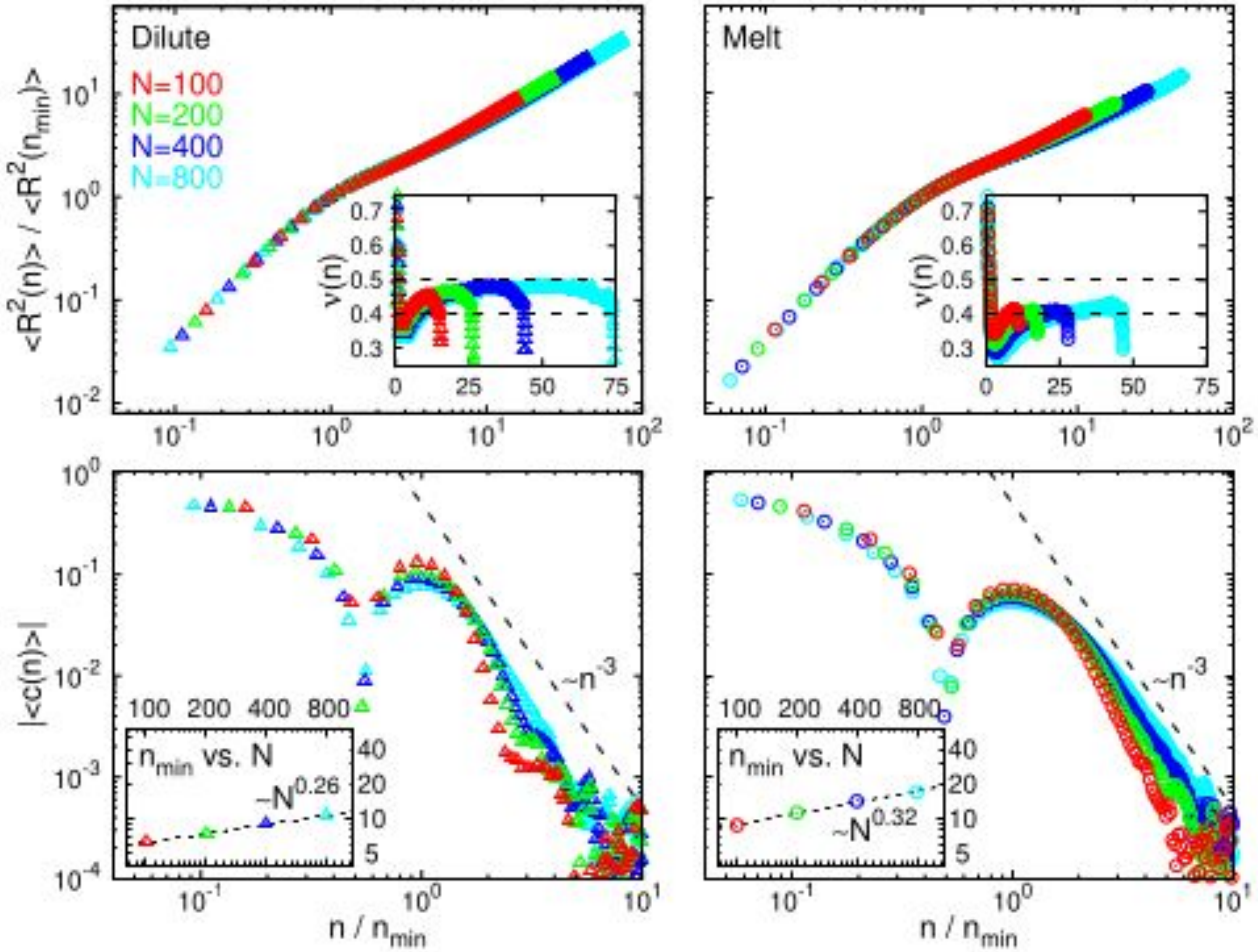


$$\langle c(n)\rangle \equiv \frac{\langle \vec{t}_{n'+n}\cdot\vec{t}_{n'}\rangle}{\langle \vec{t}_{n'}^{\,2}\rangle},$$

$$n_{min}(Pe, N)$$

M.A. Ubertini, E.Locatelli, A. Rosa, arXiv:2404.08425 (submitted)

Melts of Active Linear Chains



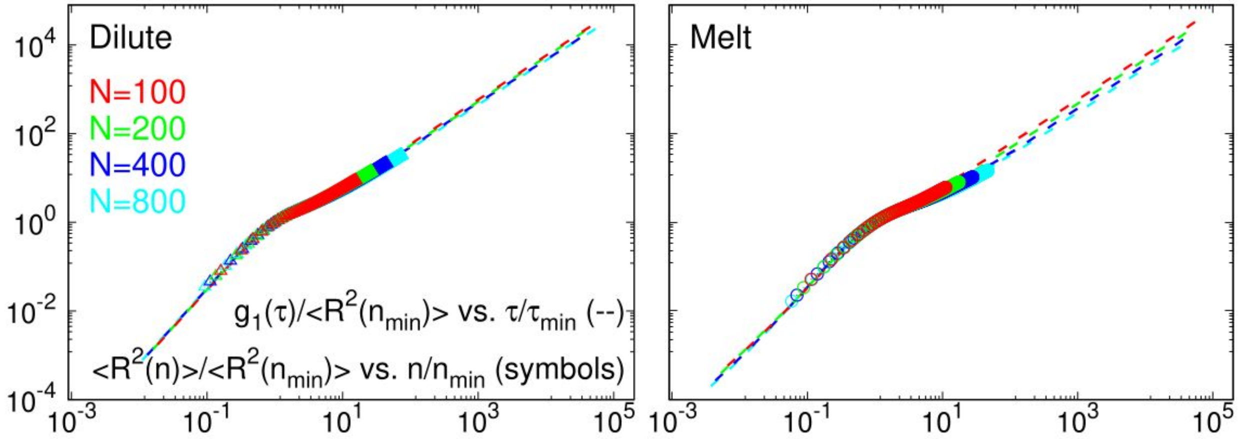
$n_{min}(Pe, N)$ is the length that marks the minimum of the tangent correlation function.

It is a characteristic length scale of the system both at infinite dilution and in the melt.

M.A. Ubertini, E.Locatelli, A. Rosa, arXiv:2404.08425 (submitted)

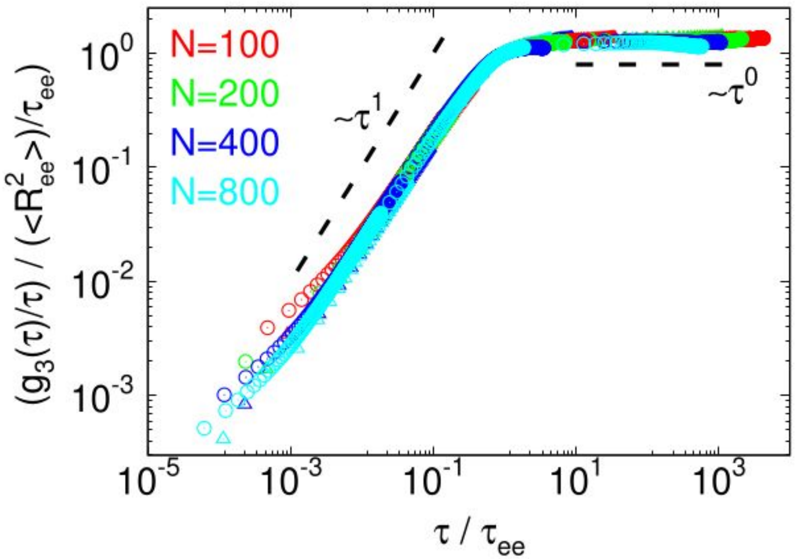
Melts of Active Linear Chains

Dynamics: two different length scales



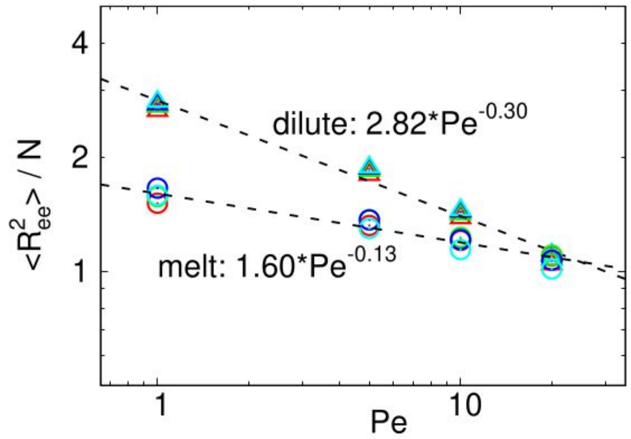
$n_{min}(Pe, N)$ is the characteristic scale of the monomer dynamics

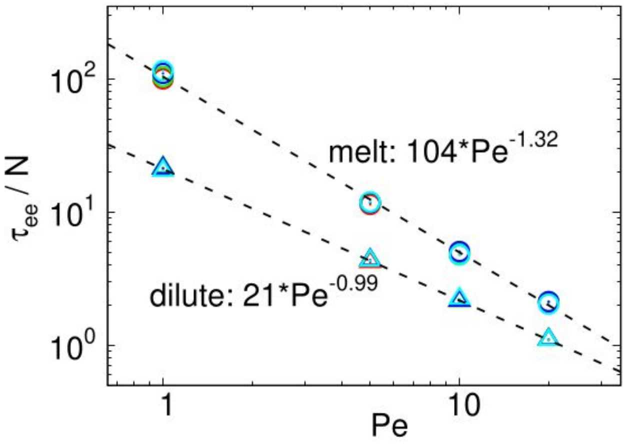
Instead, R^2_{ee} is the characteristic scale of the centre of mass dynamics, with a characteristic time scale τ_{ee}

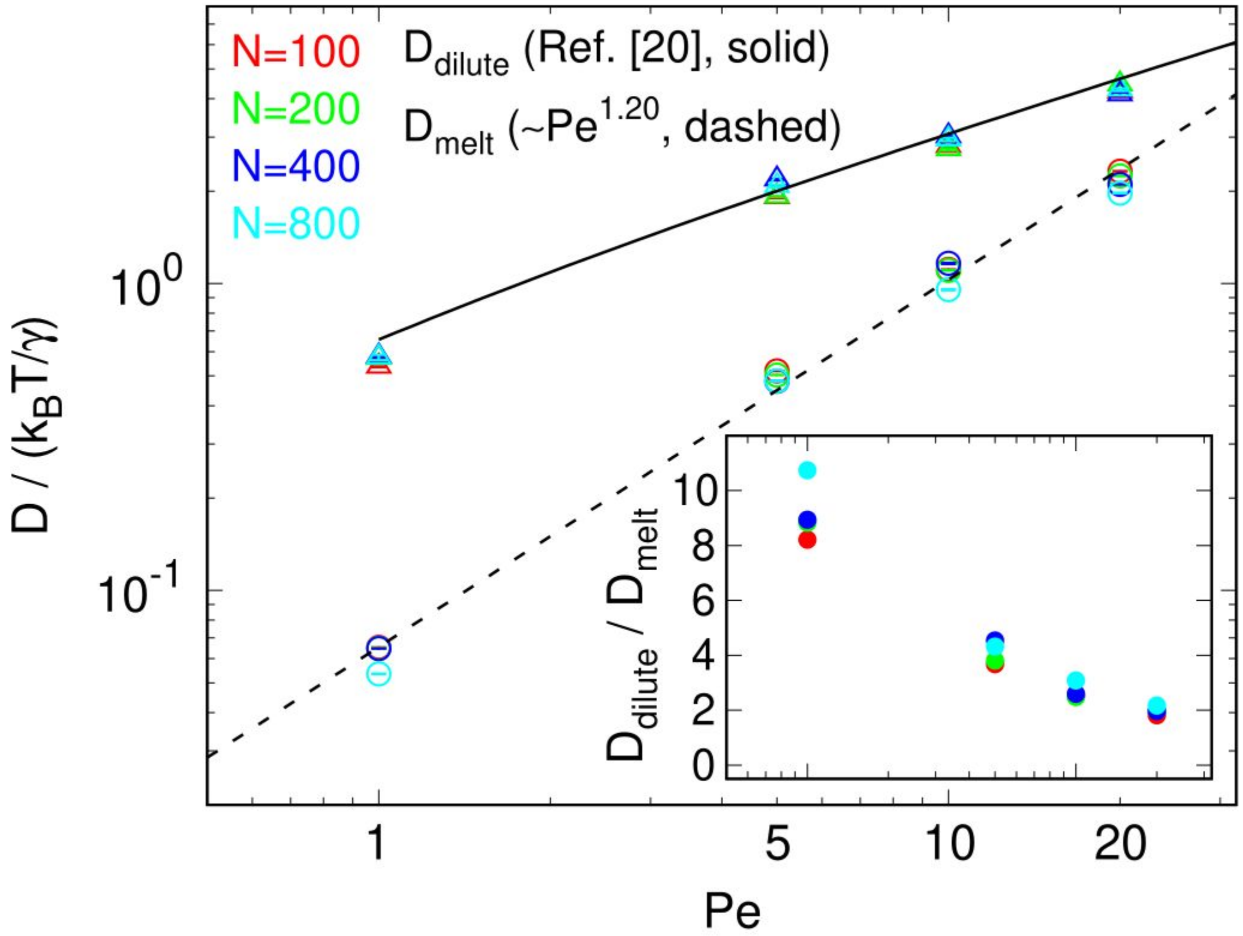


M.A. Ubertini, E.Locatelli, A. Rosa, arXiv:2404.08425 (submitted)

Melts of Active Linear Chains

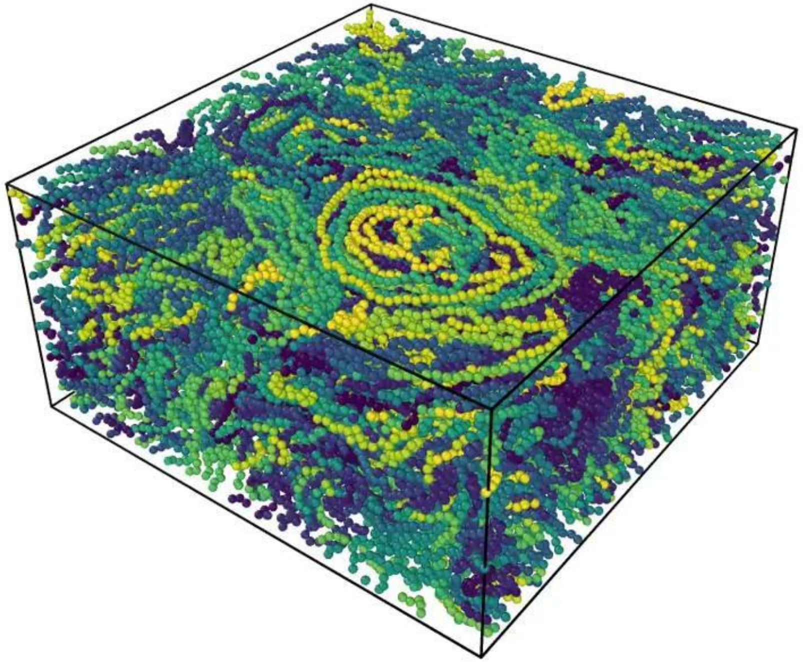






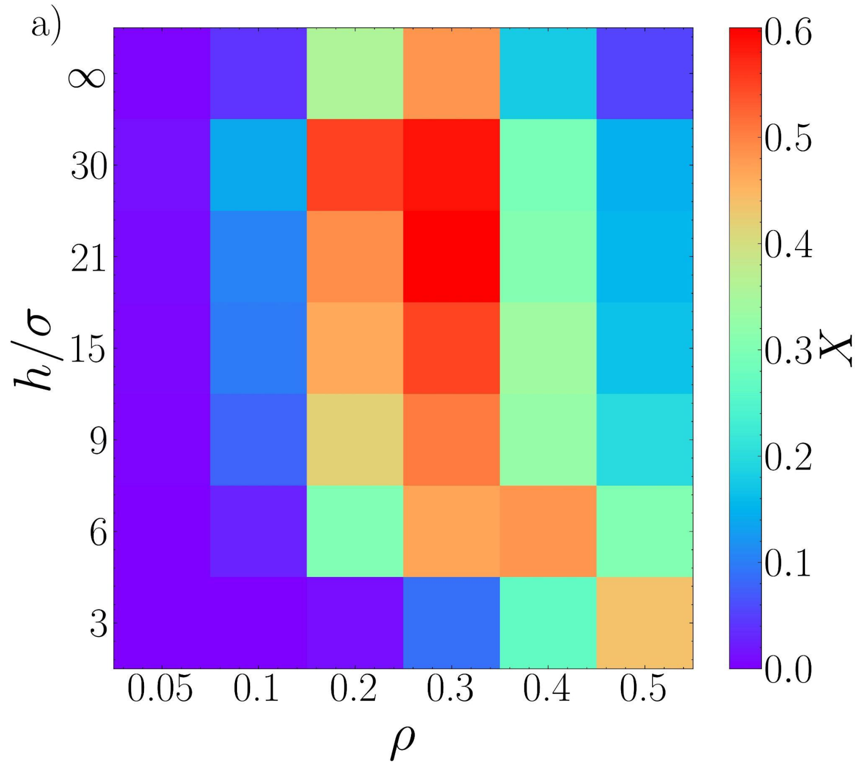
M.A. Ubertini, E.Locatelli, A. Rosa, arXiv:2404.08425 (submitted)

Active Rings under confinement

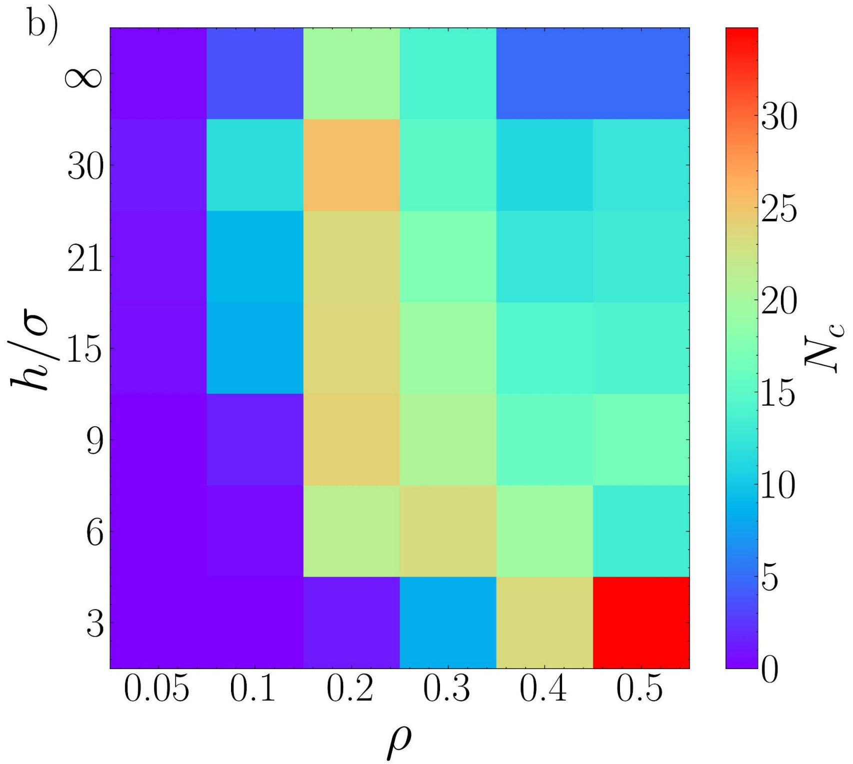


J.P. Miranda, E.Locatelli, C. Valeriani, JCTC, 2023

Active Rings under confinement



Fraction of clustered rings X



Number of clusters N_c

There is a rather large area of the ϱ-h plane in which these bundles form; too high density suppresses organization

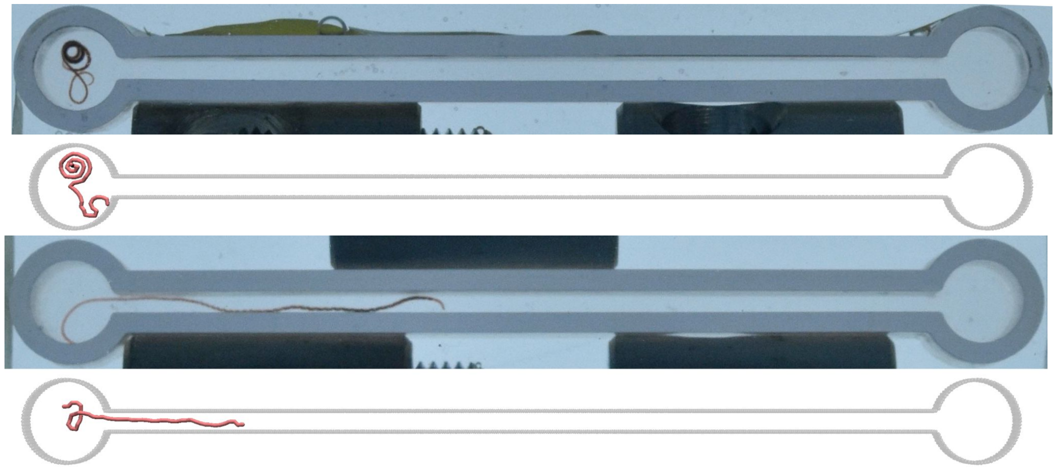
J.P. Miranda, E.Locatelli, C. Valeriani, JCTC, 2023

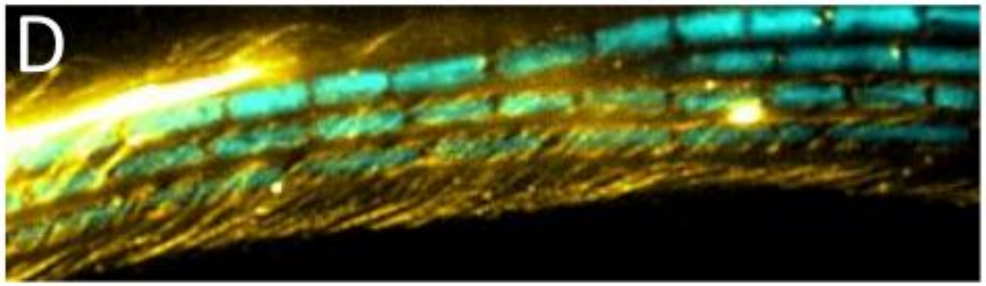
Outline

Polar Active Polymers

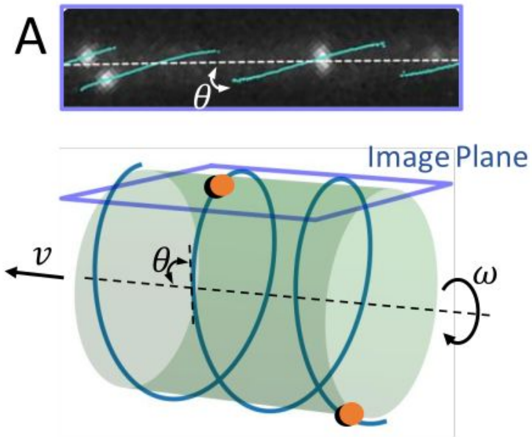
Multi-scale analysis of dense suspensions

Towards modeling biophysical systems

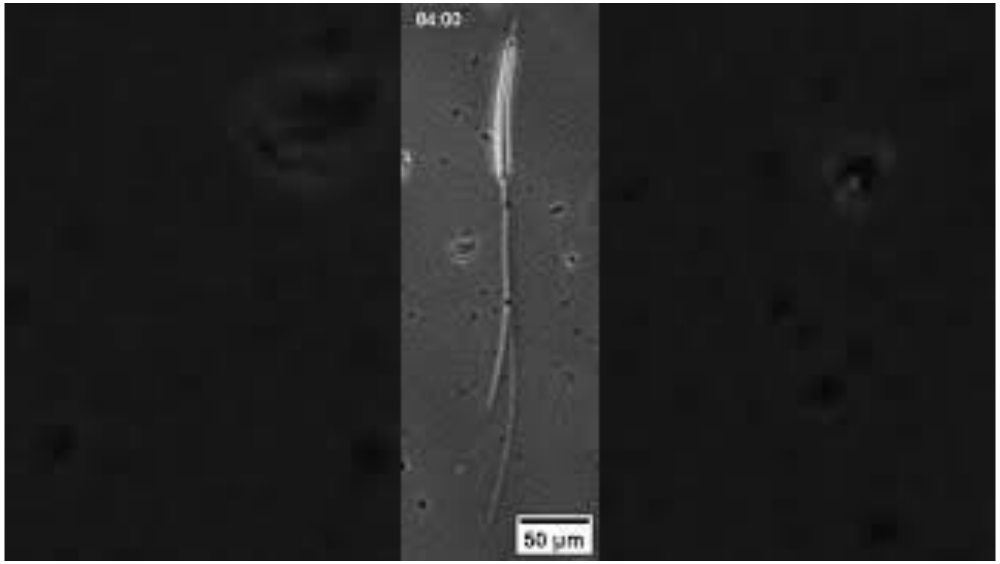




Cyanobacteria reversals

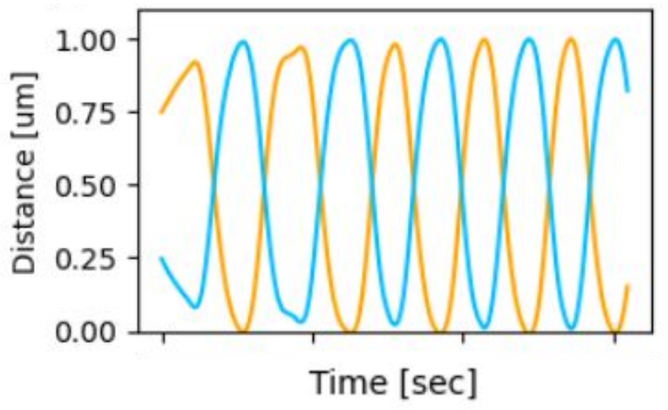


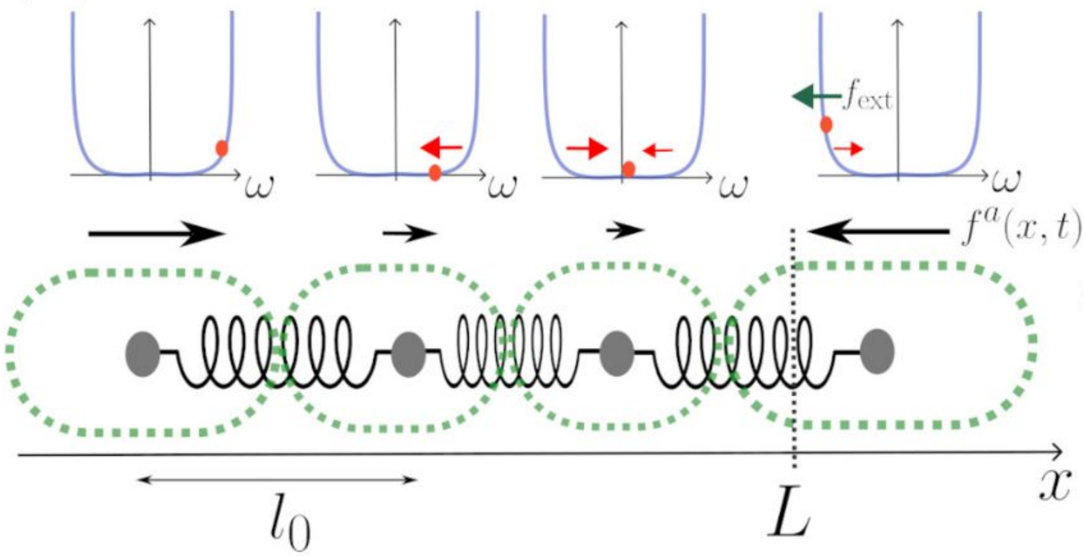
Can we come up with a (local) model for the mechanism of reversals?



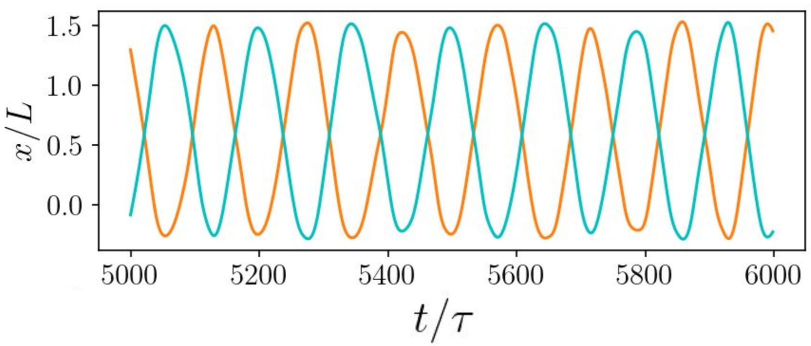
J. Rosko, K. Cremin, E.Locatelli, et al, bioRxiv, 2024.02. 06.579126

Cyanobacteria coordination model





Local (mechanical) sensing mechanism drives coordination

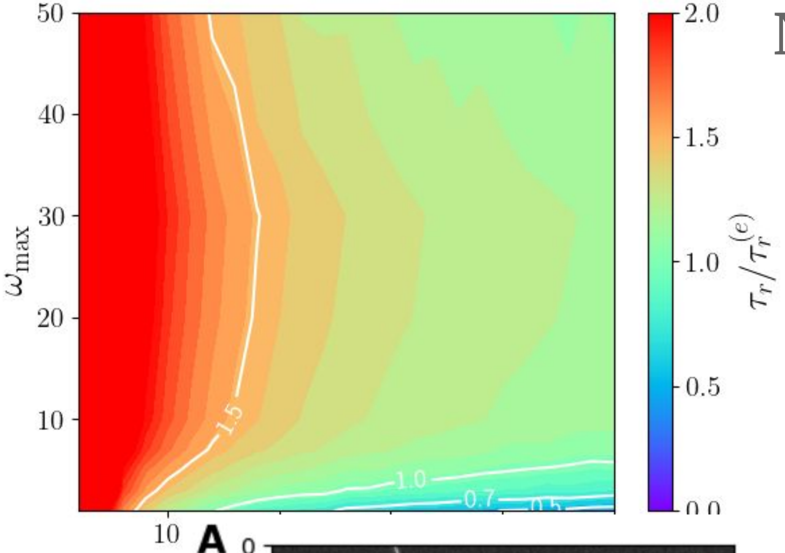


$$\dot{x}_i = \frac{1}{\gamma}\left(-\frac{dV}{dx_i} + f_i^a \cdot s_i(x,t)\right) + \xi_i(t)$$

$$\dot{\omega}_i(x,t) = \frac{1}{\gamma_\omega}\left(-\frac{dU_c}{d\omega_i} - \frac{dV_\omega}{dx_i} + f_{\rm ext}(x,t)\right) + \eta_i(t)$$

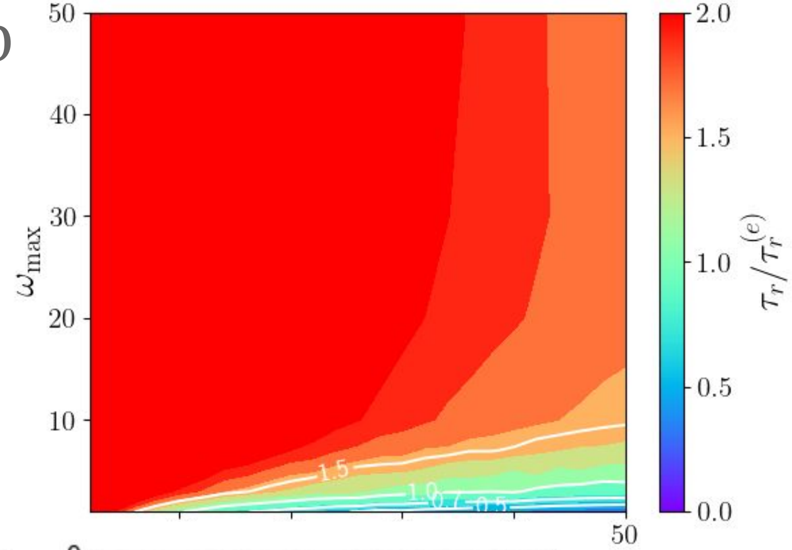
J. Rosko, K. Cremin, E.Locatelli, et al, bioRxiv, 2024.02. 06.579126

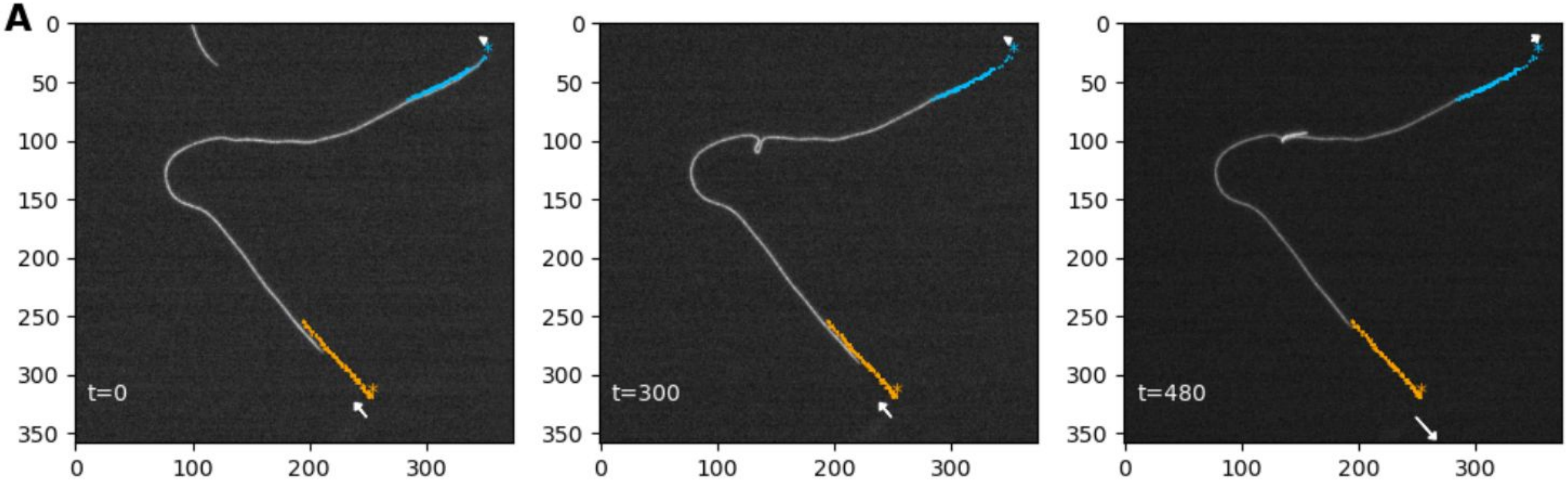
Cyanobacteria coordination model



N=10

N=50

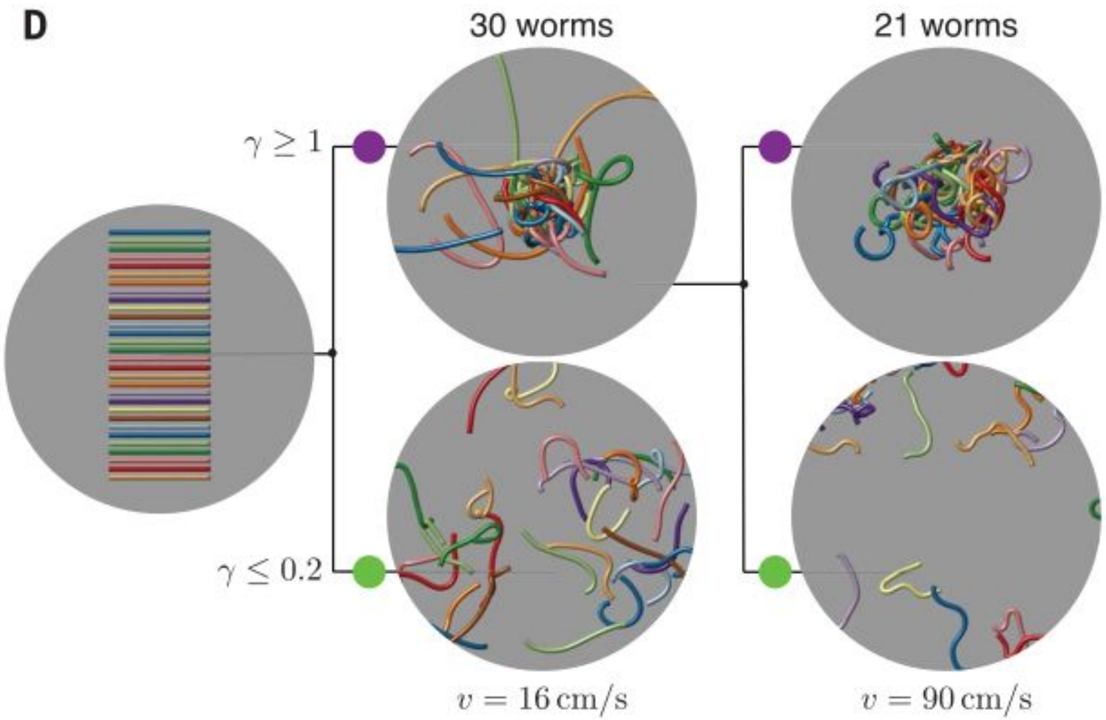




J. Rosko, K. Cremin, E.Locatelli, et al, bioRxiv, 2024.02. 06.579126

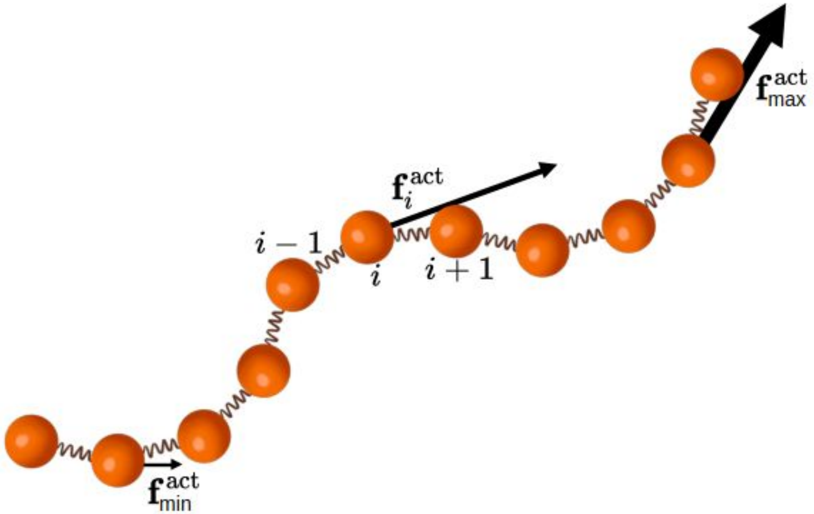
Modeling worms under confinement

Science 380, 392–398 (2023)

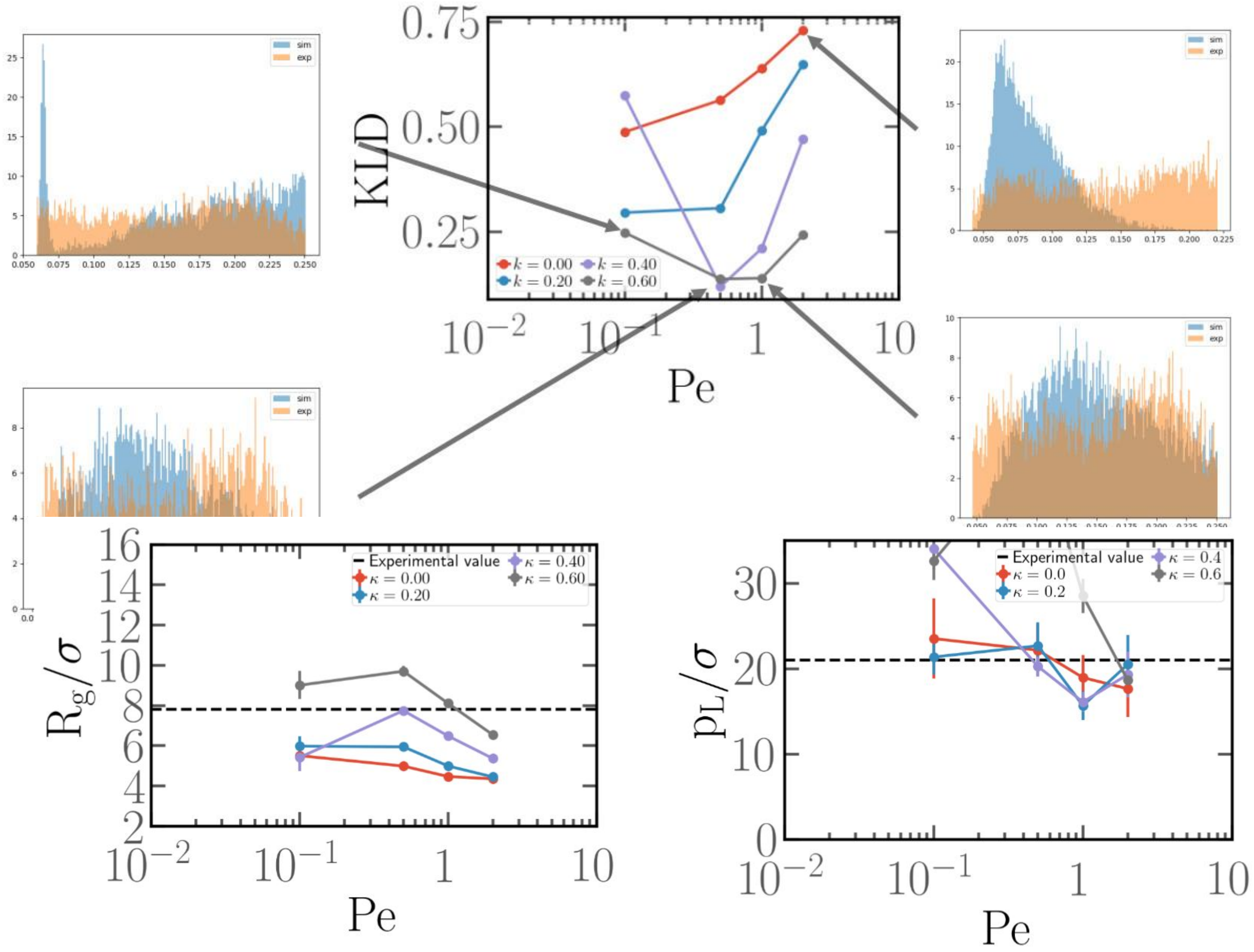


Does a simpler (and more transferable) model exists?

Modeling worms under confinement



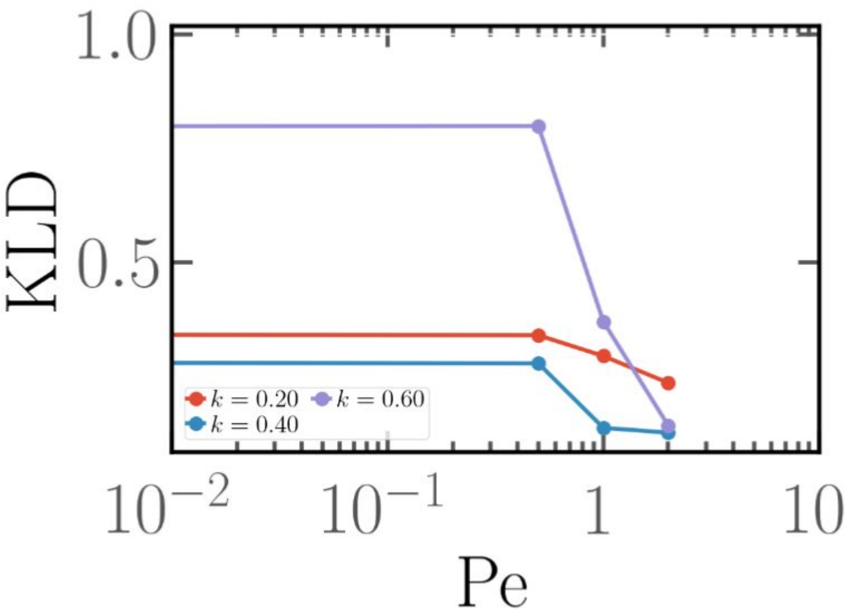
Bulk

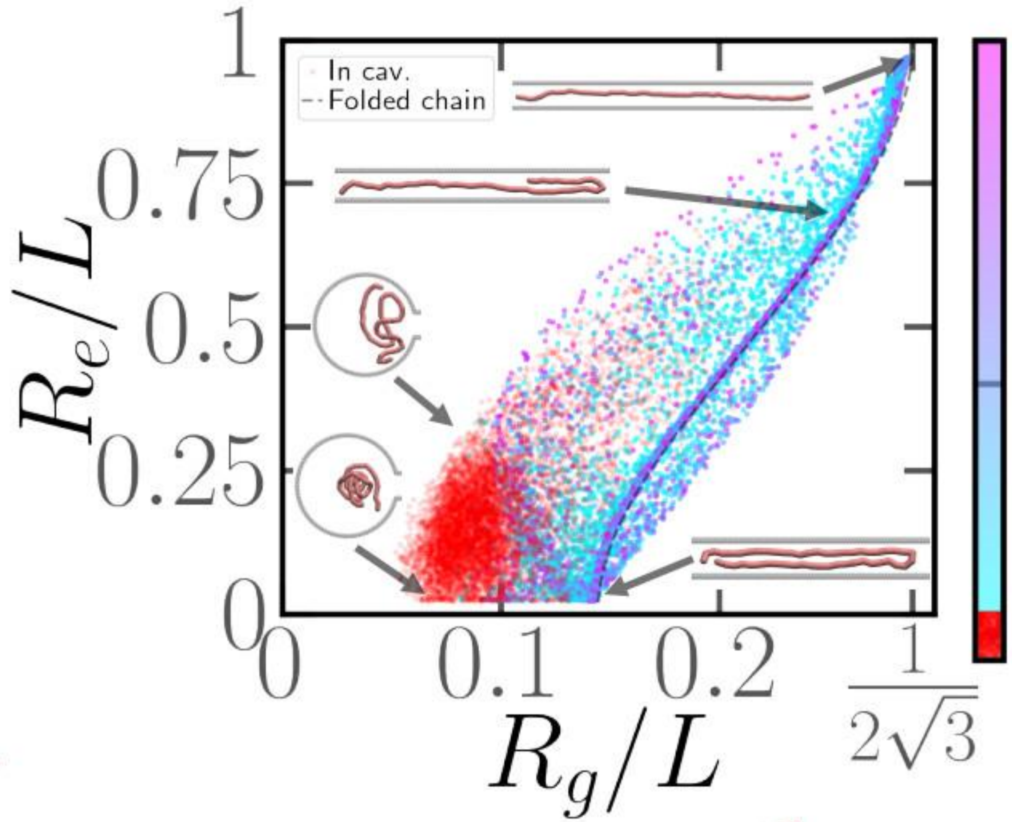


Semi-flexible polymer
Non-homogeneous activity profile
3D+gravity

Modeling worms under confinement

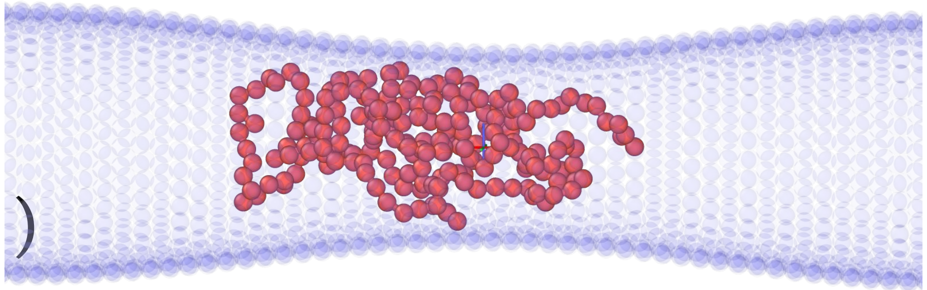
Confinement





Perspectives

- Linear polymers in cylindric and corrugated channels
(Phys. Rev. Lett. 131, 048101 (2023))



- Non-homogeneous activity

- Knots & entanglements

- Multi-scale modeling micro/macro-organisms
    - 3D model of reversing bacteria (plectoneme formation)
    - assembly of bacteria (effect of external bias)
    - learning the worm model

Acknowledgments

Collaborators

V. Bianco (UCM)
P. Malgaretti (Helmholtz Institute Erlangen)

C. Valeriani, J. P. Miranda, J. Martin Roca (UCM)

C. N. Likos (Univie)
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S. Kundu, M. Ubertini, A. Rosa (SISSA)

O. Soyer (Warwick), M. Polin (IMEDEA)

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@elocatelli86

http://statphys.dfa.unipd.it/people/locatelli.php

TECHNISCHE UNIVERSITÄT WIEN
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