Tales of tails

Elastohydrodynamics of microscale (loco)motion

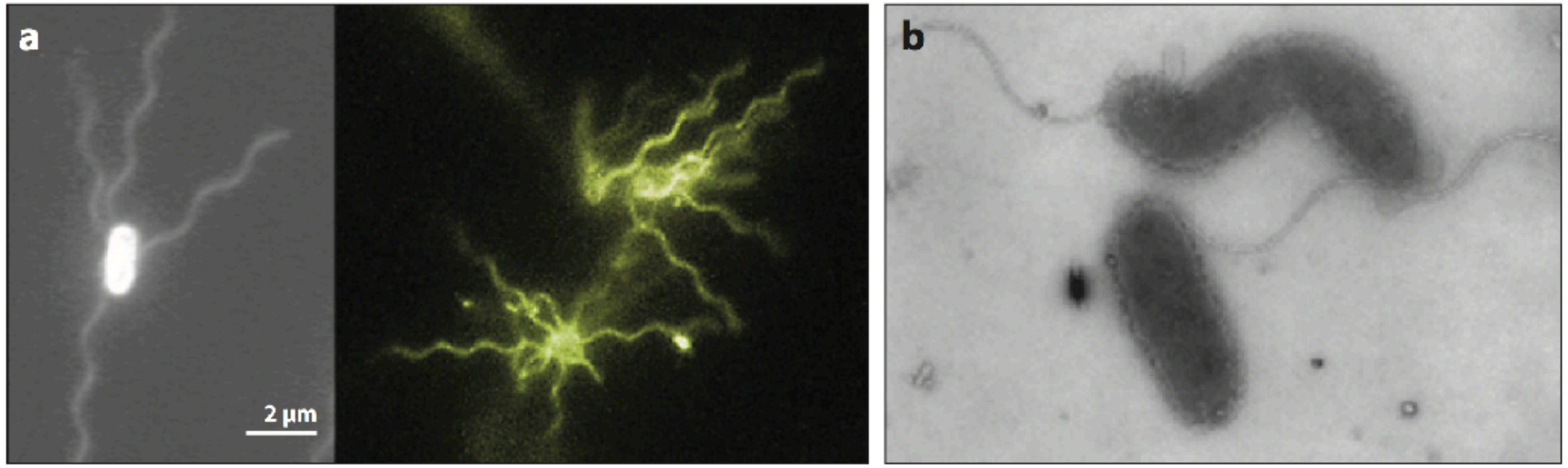
Maciej Lisicki

UNIVERSITY
OF WARSAW

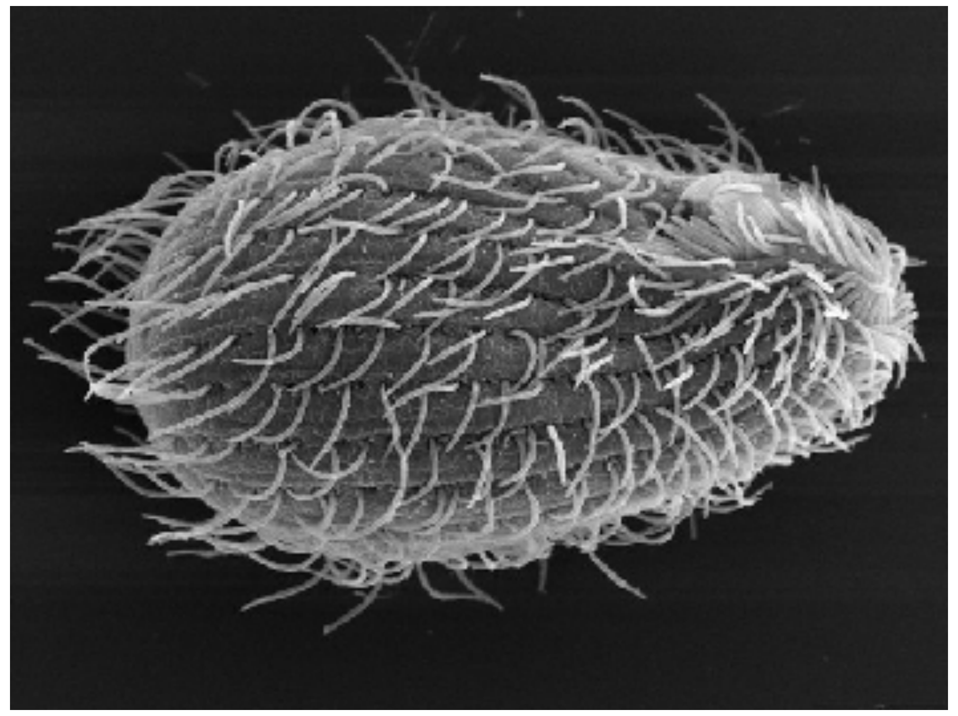
How do microorganisms move?

Peritrichous
Escherichia coli

Polar monotrichous
Pseudomonas aeruginosa



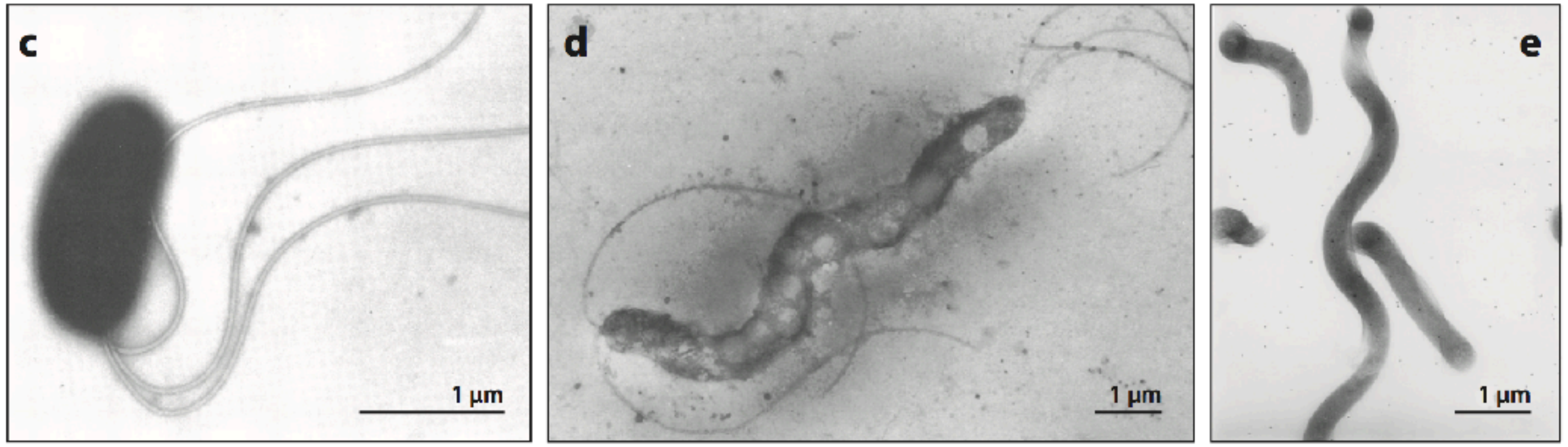
Tetrahymena thermophila



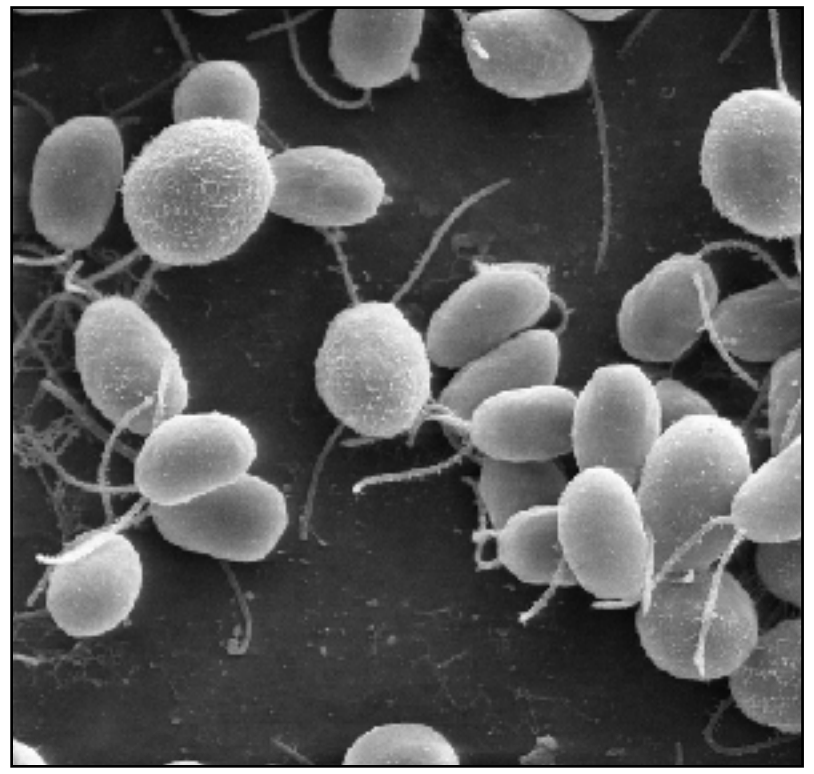
Polar lophotrichous
Photobacterium fischeri

Polar amphitrichous
Ectothiorhodospira halochloris

Spirochetes with endoflagella
Borrelia burgdorferi



Chlamydomonas reinhardtii



Lauga (2016)

Variety of shapes and swimming gaits

Different morphology & physiology: prokaryotes vs eukaryotes

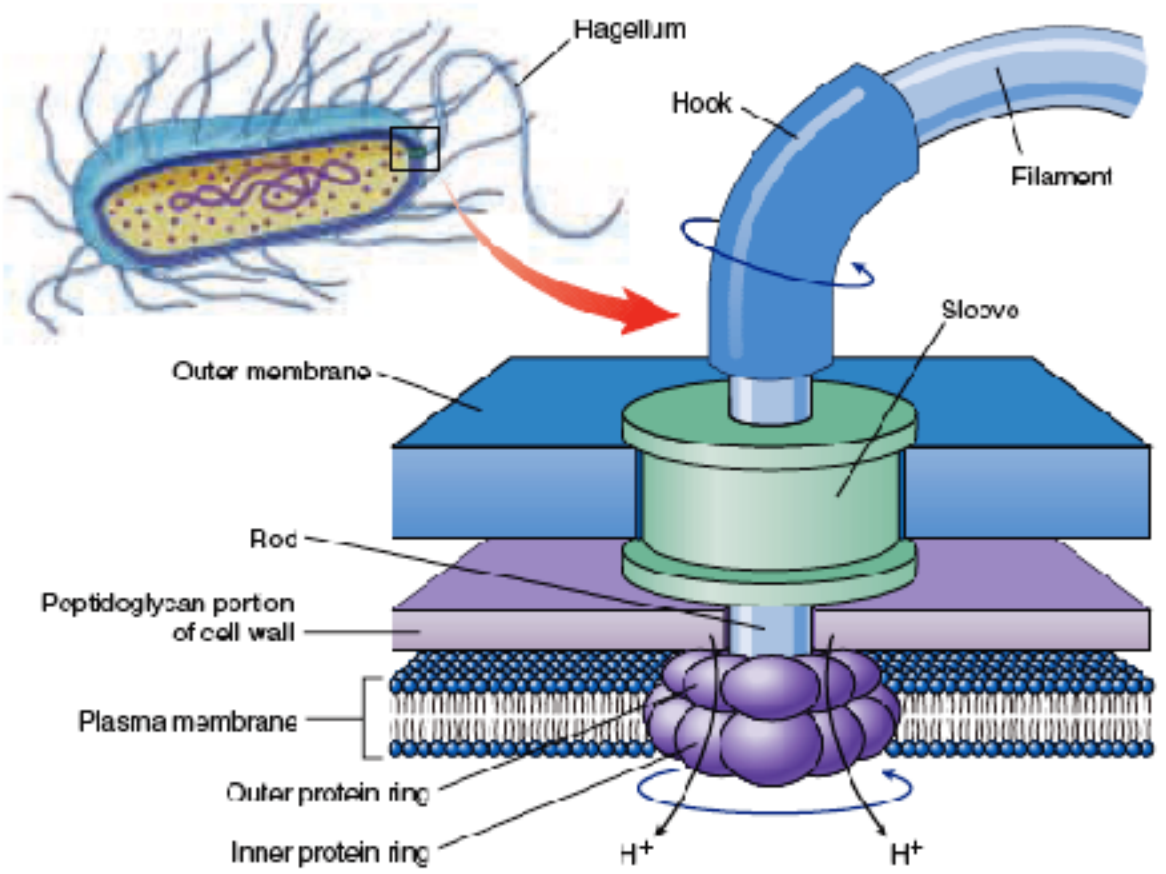
Prokaryotic vs. eukaryotic flagella

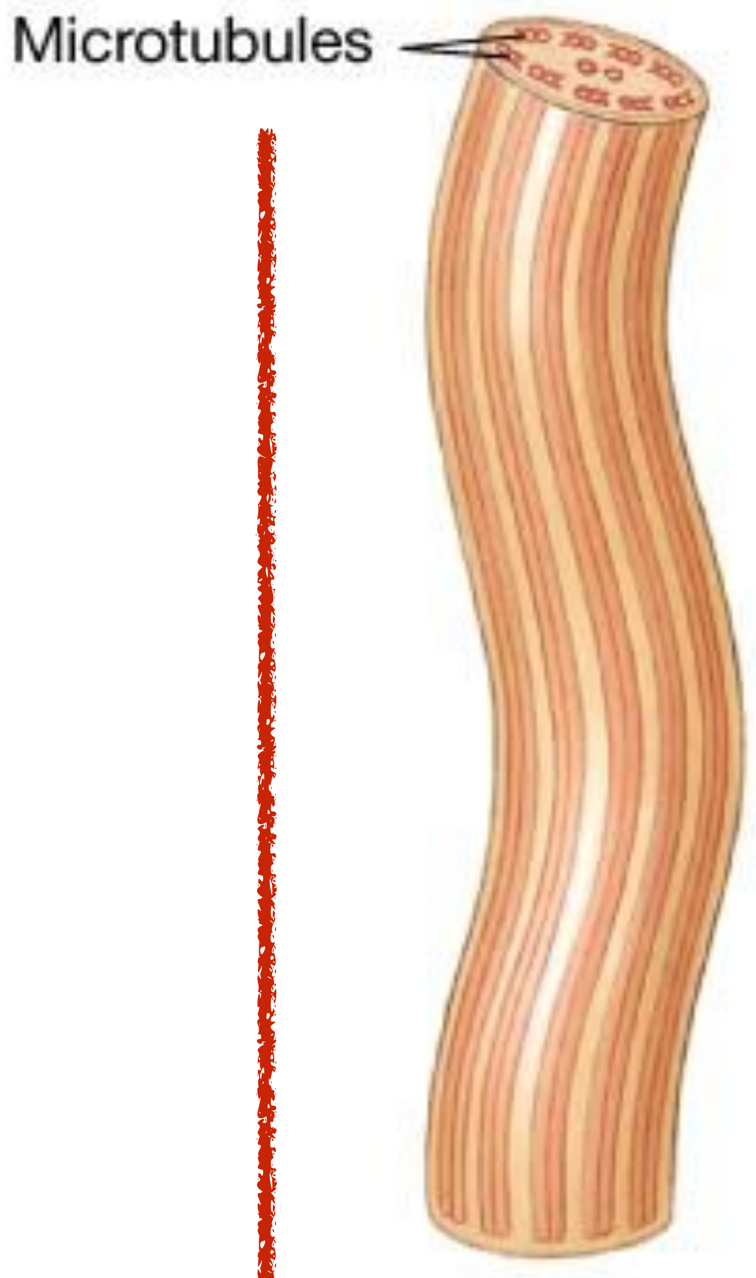
Bacteria
Archaea

Passive flagella

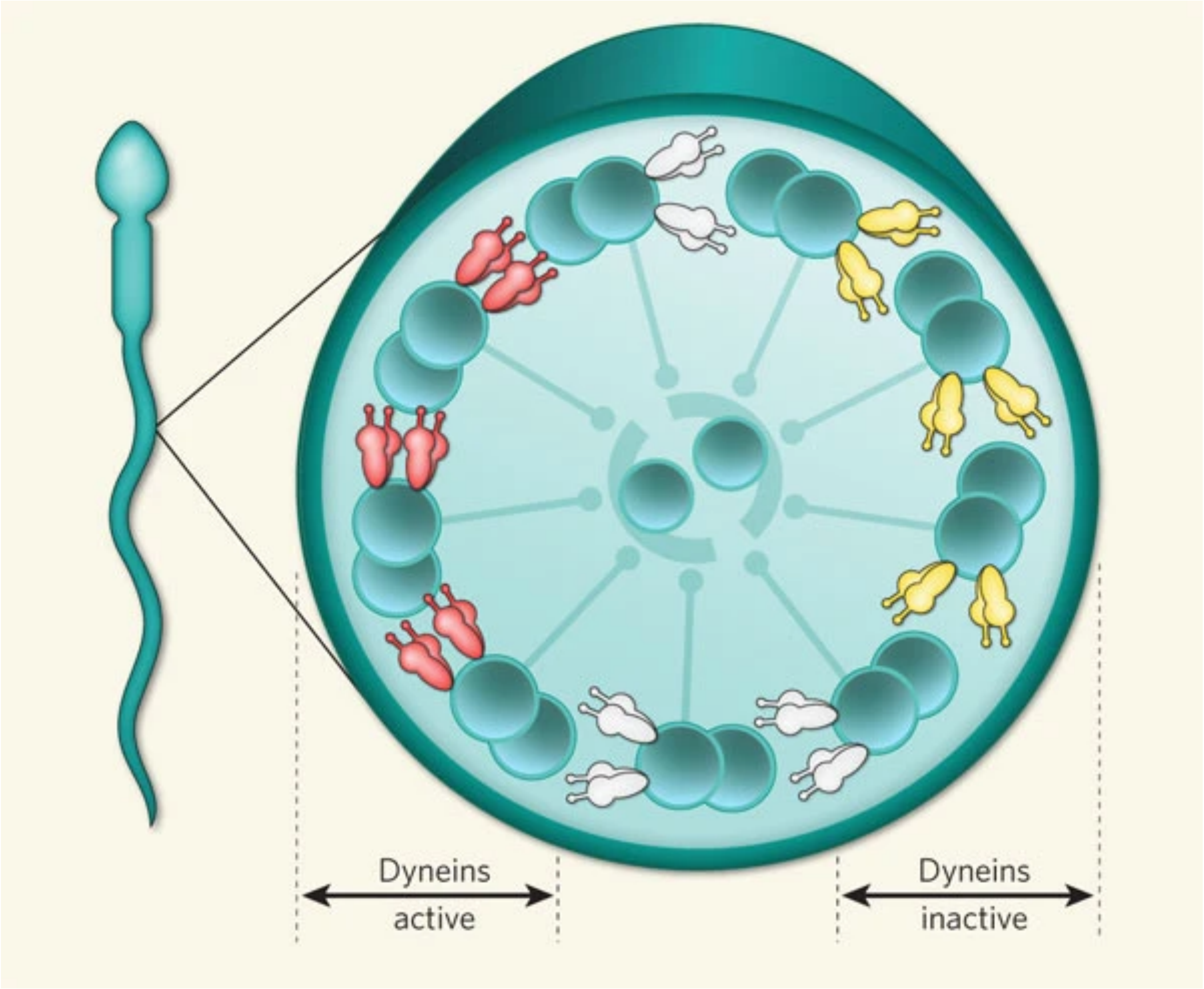
Prokaryotic flagellum

http://env.boblupo.com/AP-Lectures/





Eukaryotic flagellum

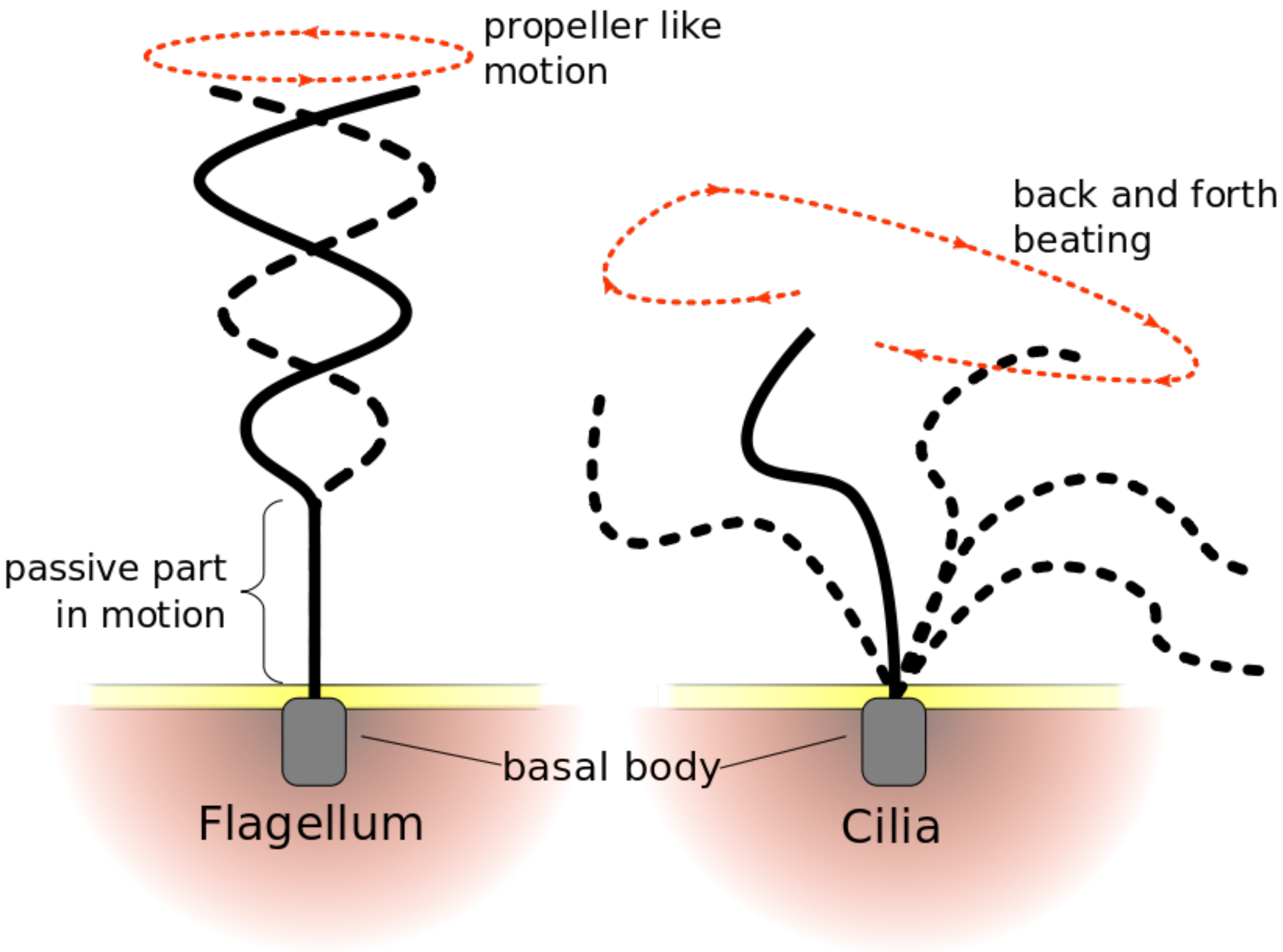


Mitchison & Mitchison *Nature* (2010).

Algae
Ciliates
Sperm cells
etc.

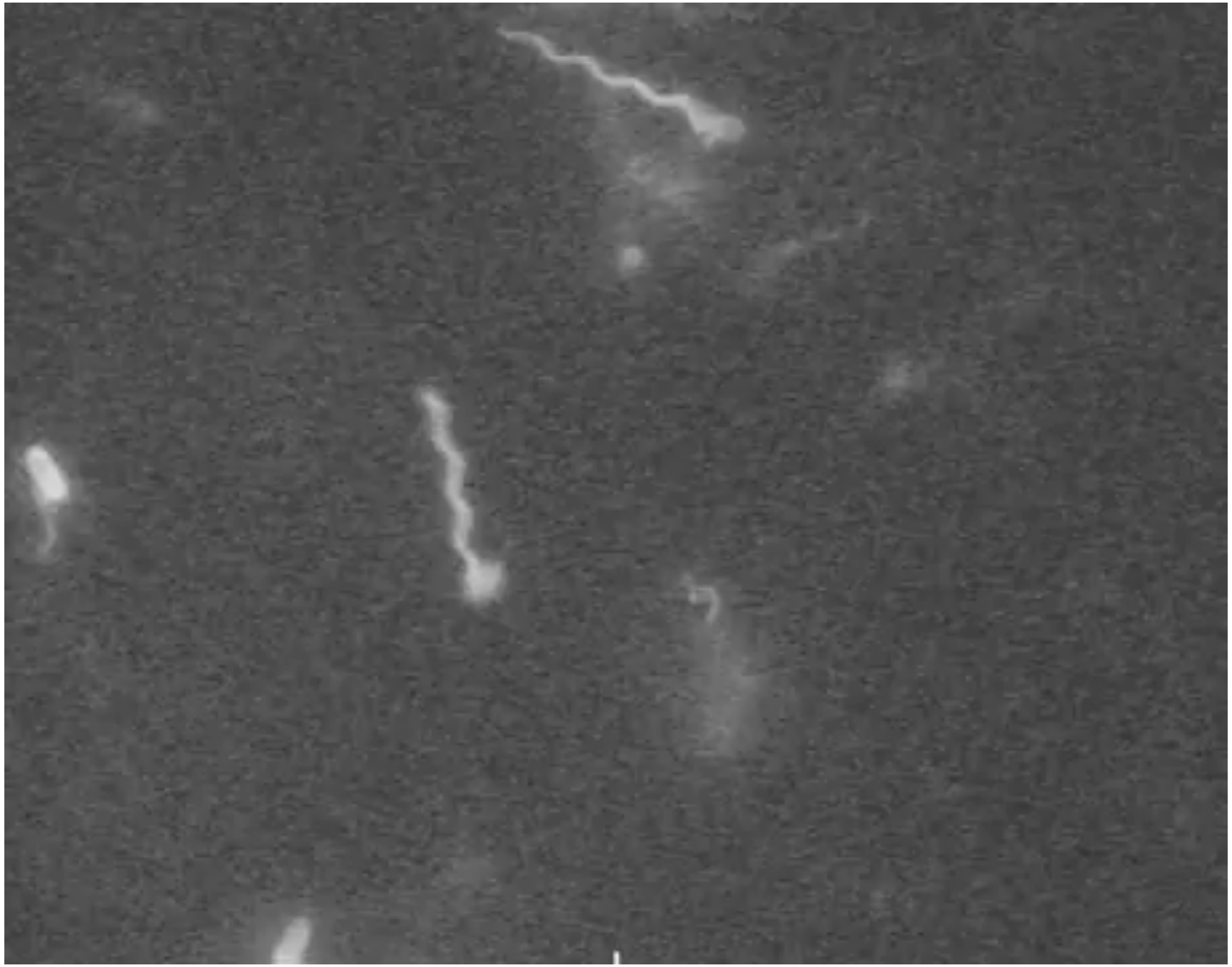
Active flagella

Different beating patterns



L. Kohidai, Wikipedia

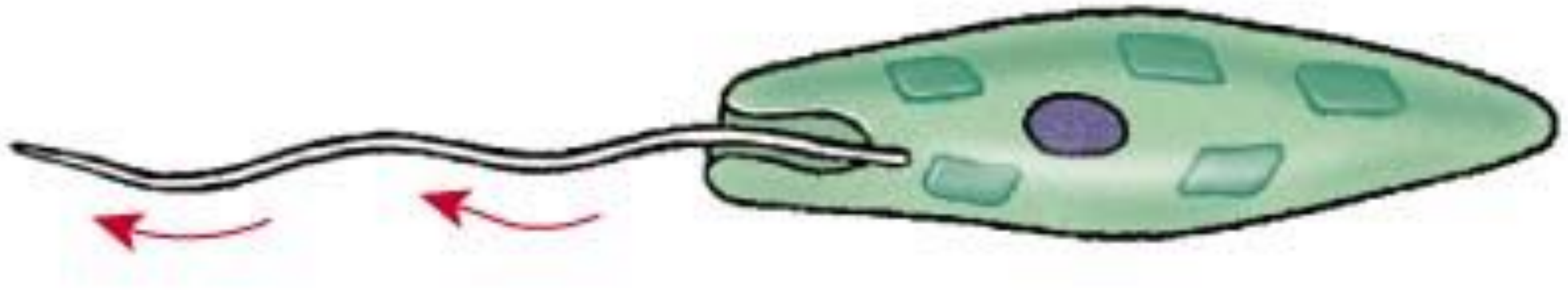
Prokaryotes – *E. coli* in motion

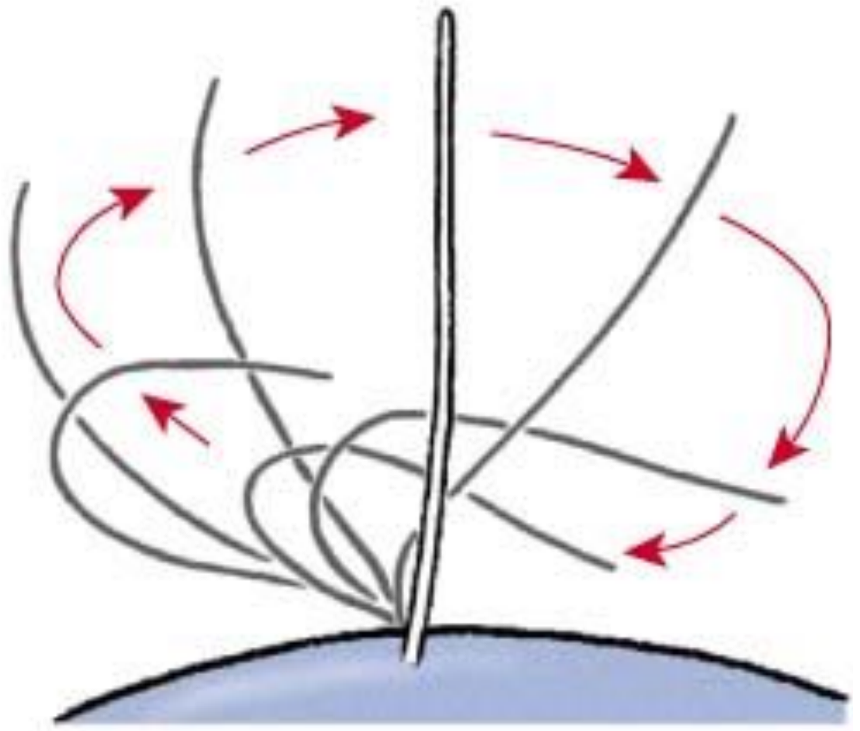


Howard Berg, Harvard University

Eukaryotes – ciliary beating

Multiple (active) beating patterns





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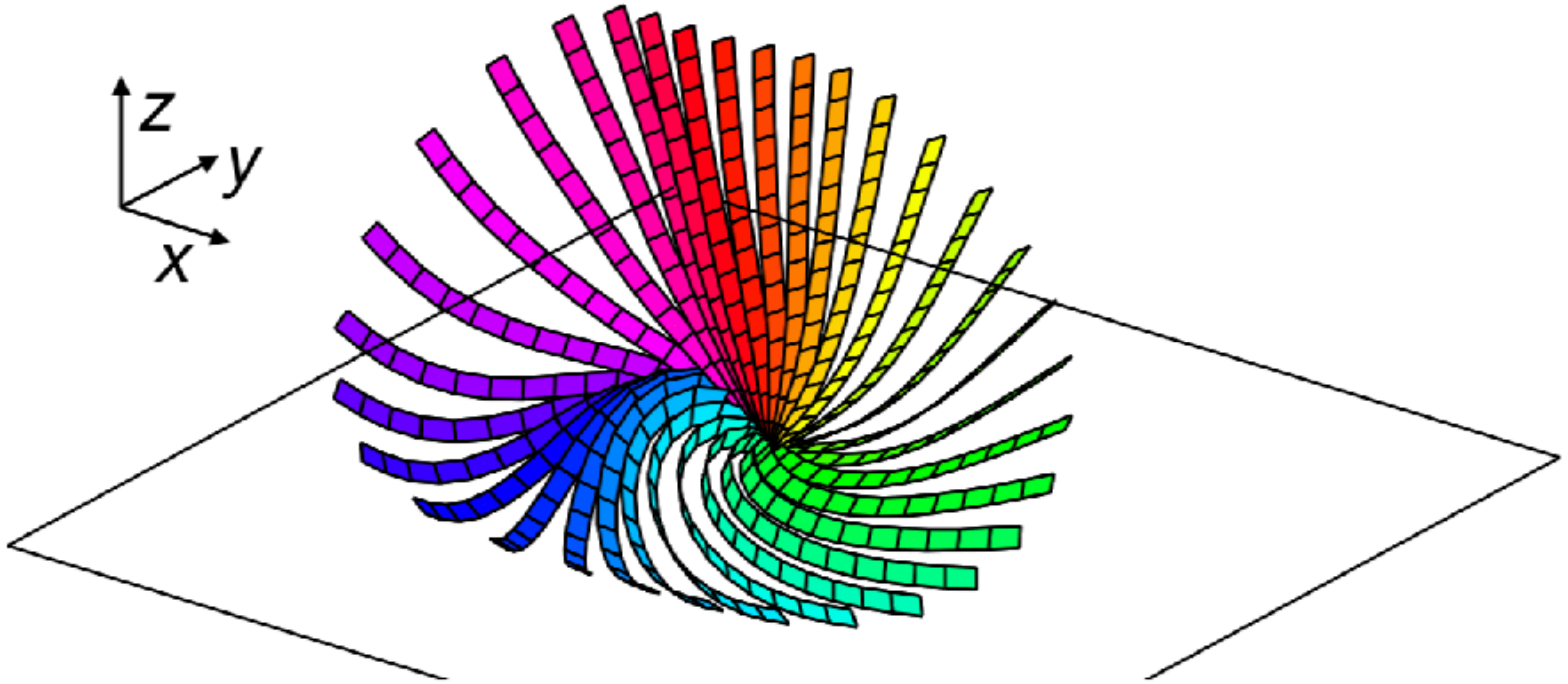
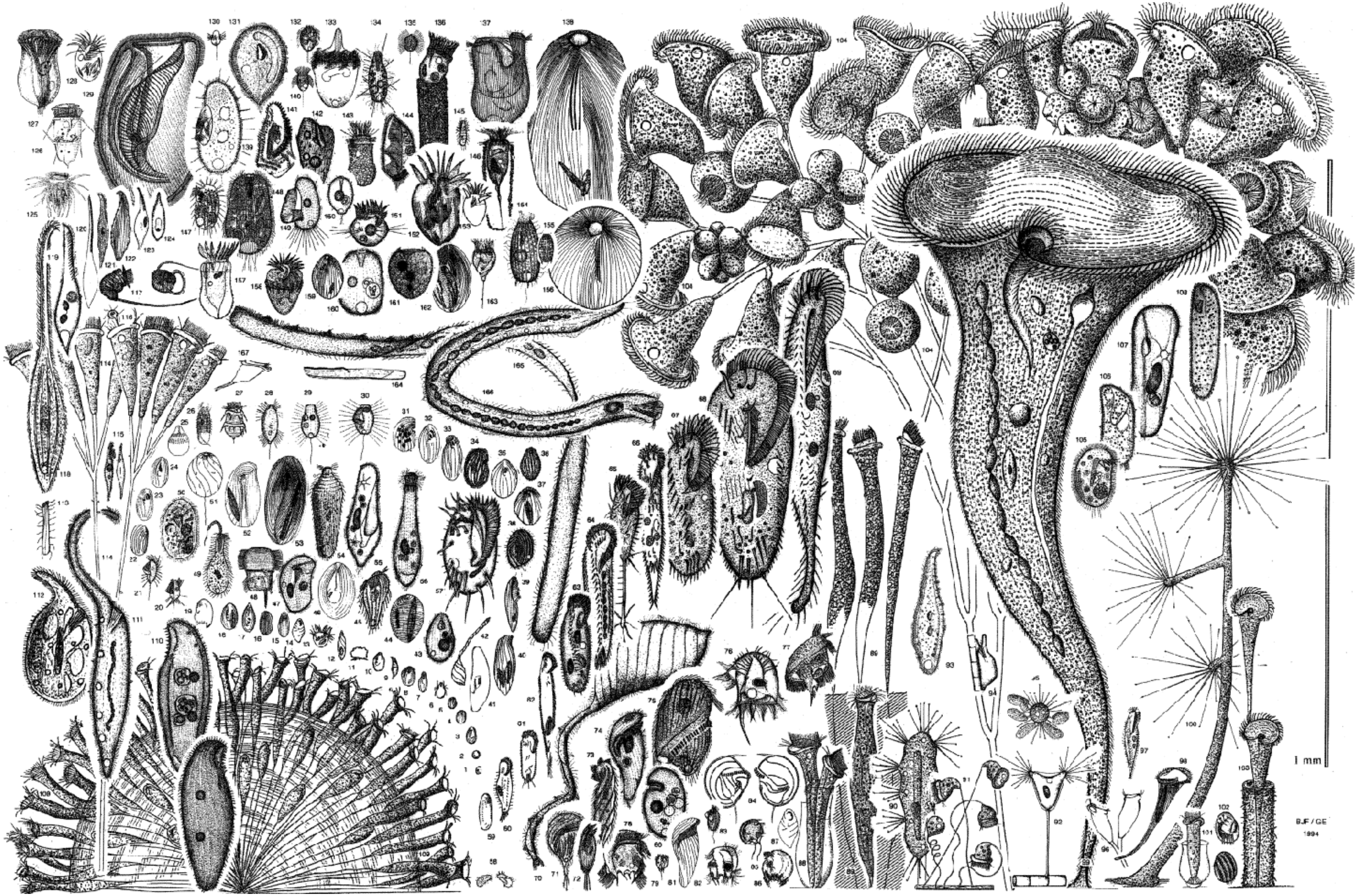


Eloy & Lauga (2012)

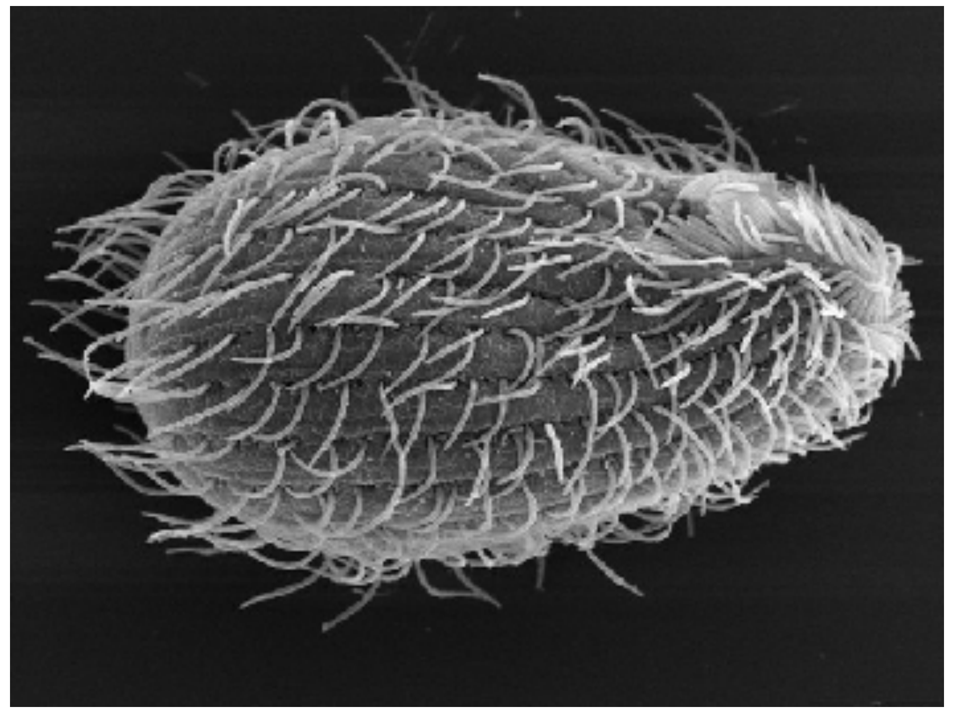
Power stroke – recovery stroke

Ciliates

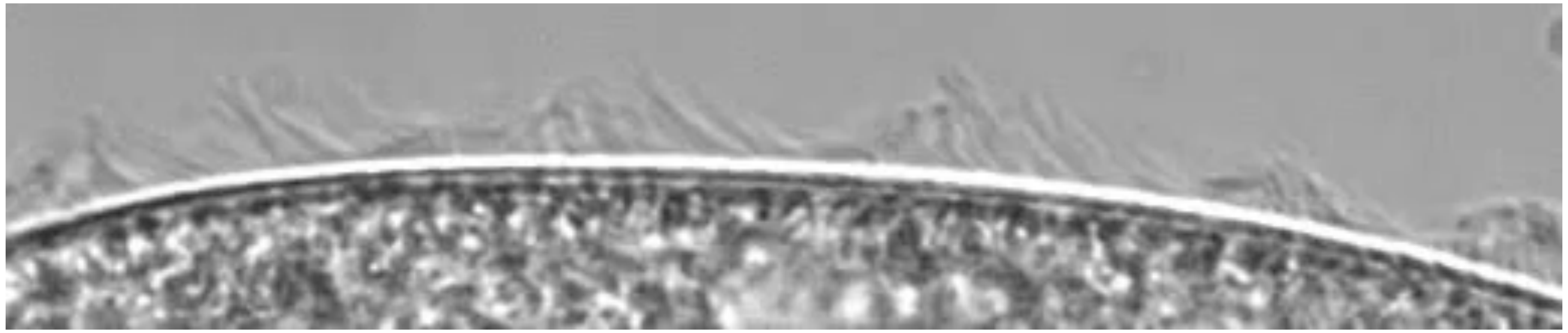


Ciliate Diversity Chart, B.J. Finlay and G.F. Esteban, Institute of Freshwater Ecology, Windermere Laboratory, UK

Ciliates: surface flow generation (swimming)



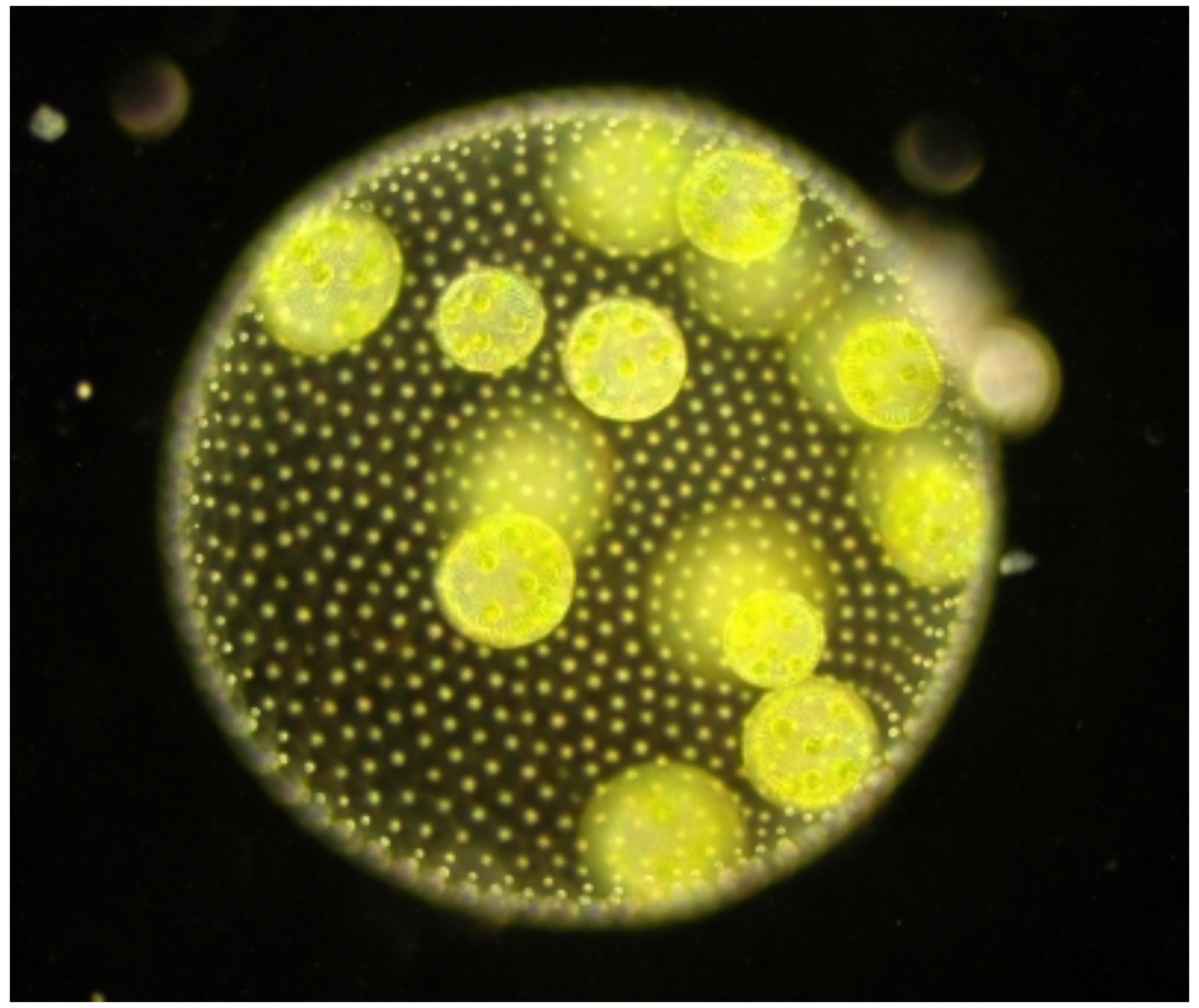
Tetrahymena thermophila

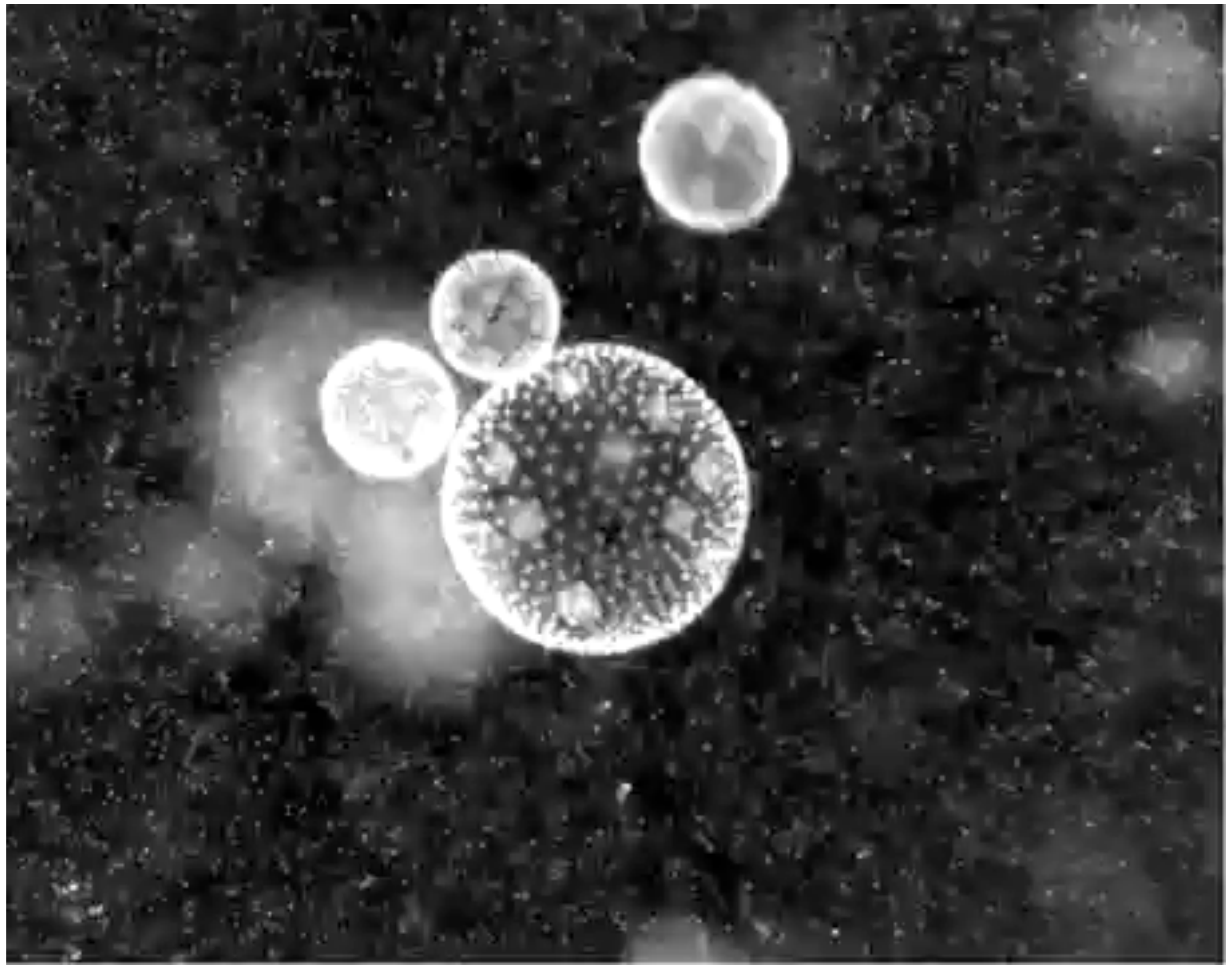


Metachronal waves

S. Acanthopagrus, youtube.com

Sizes ~ 10-1





Speeds ~ 1-

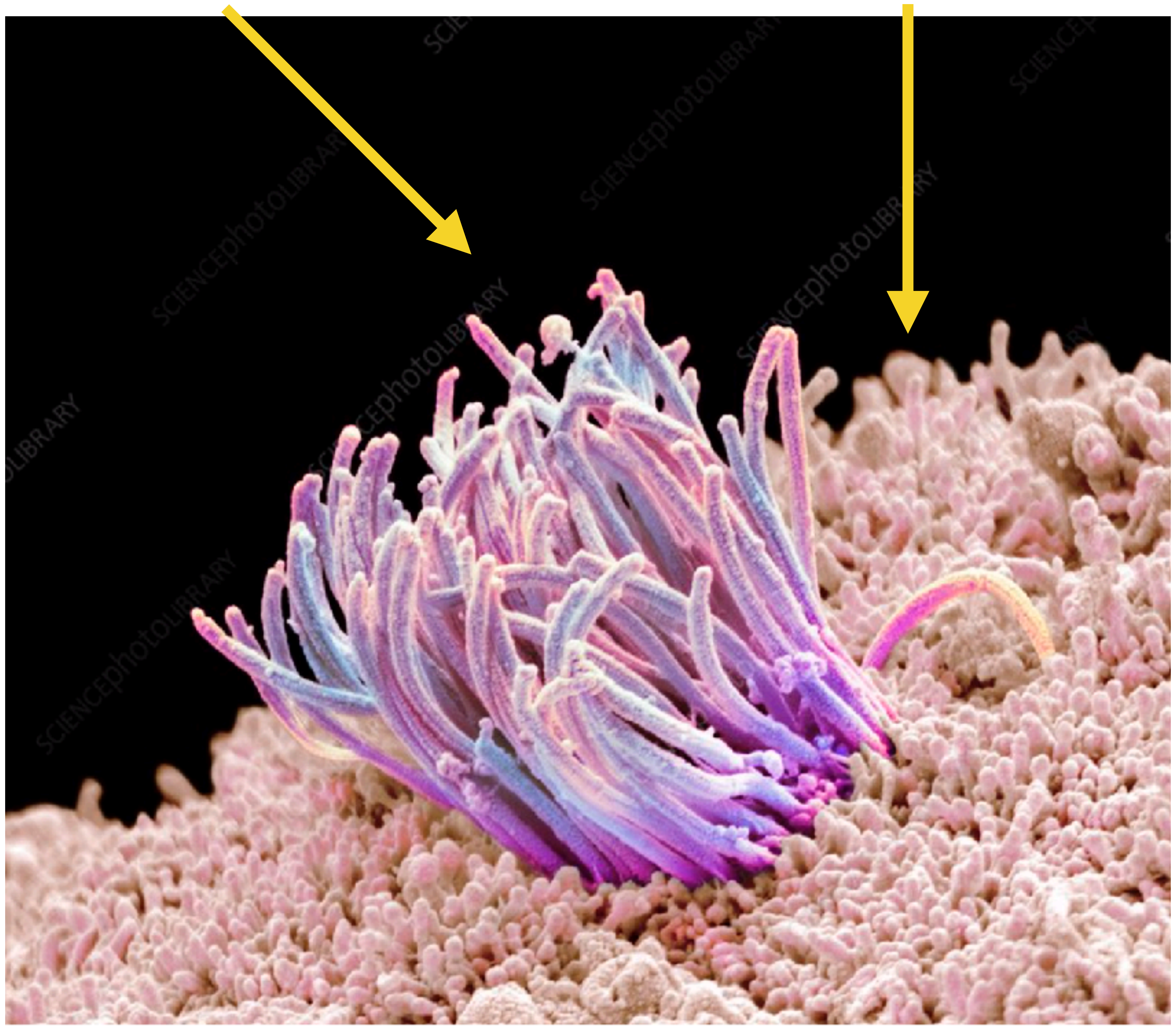
Surface flow-driven propulsion

Volvox carterii, Goldstein Lab, Cambridge

Ciliary stirring & pumping

cilia transport the mucus

secreting cells produce mucus



Inside a fallopian tube

https://www.sciencephoto.com/media/137841/view

Water, water everywhere!

MIT/ JPL

Microscale flows

Reynolds number

$$\mathrm{Re} = \frac{\rho U \ell}{\eta}$$

Characteristic length & flow velocity

Microworld: small *U* and *l*
or: large viscosity

$$\mathrm{Re} = \frac{inertia}{viscosity} \ll 1$$

G.G. Stokes

Stokes equations

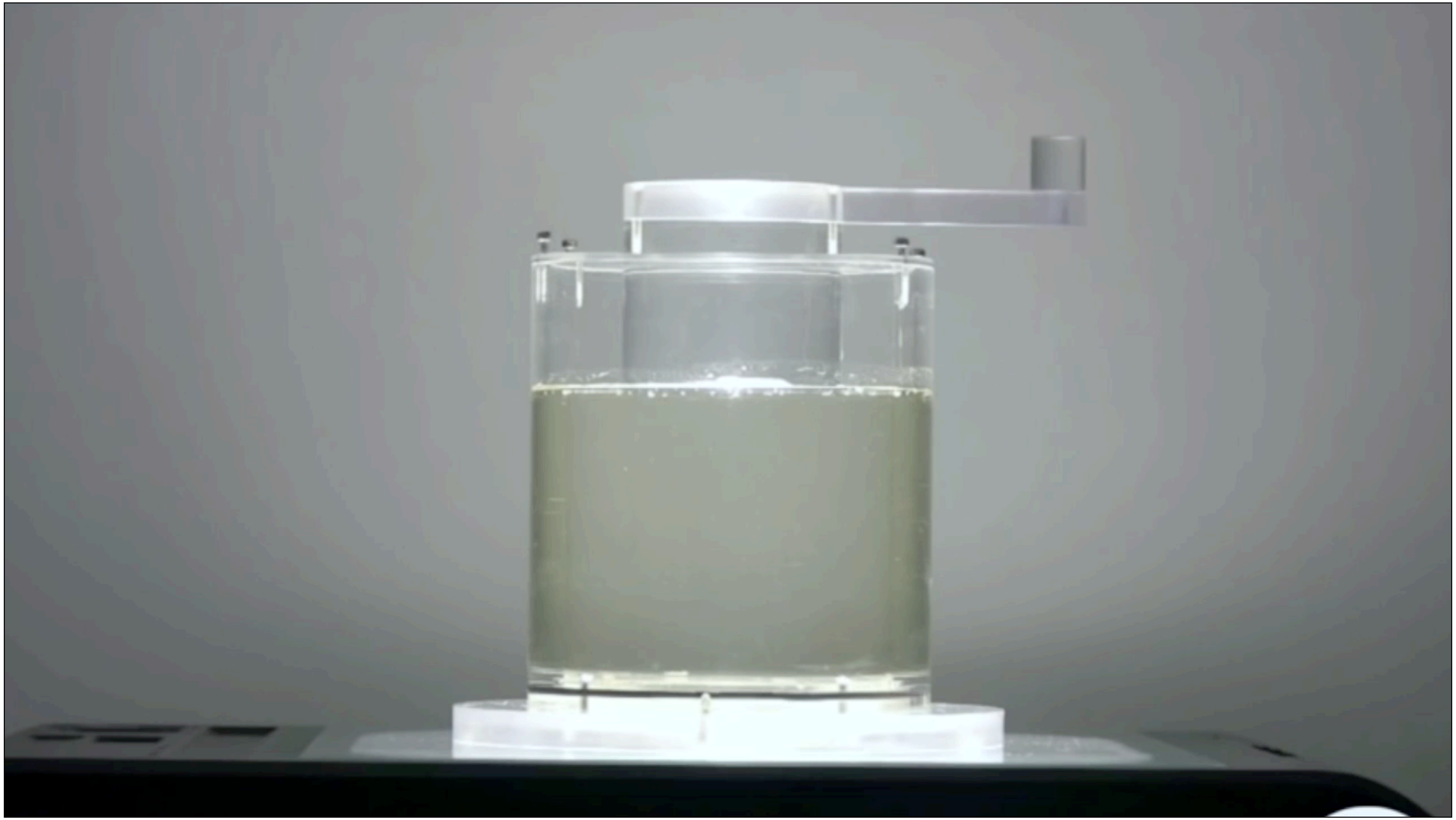
$$\begin{aligned} -\nabla p + \eta \nabla^2 \mathbf{v} &= -\mathbf{f}, \\ \nabla \cdot \mathbf{v} &= 0, \end{aligned}$$

No inertia, no turbulence!

Properties of viscous flows: Stokes flows

1. **Instantaneity (stationarity)**
2. **Constant force = constant velocity**
3. **Kinematic reversibility**

Kinematic reversibility

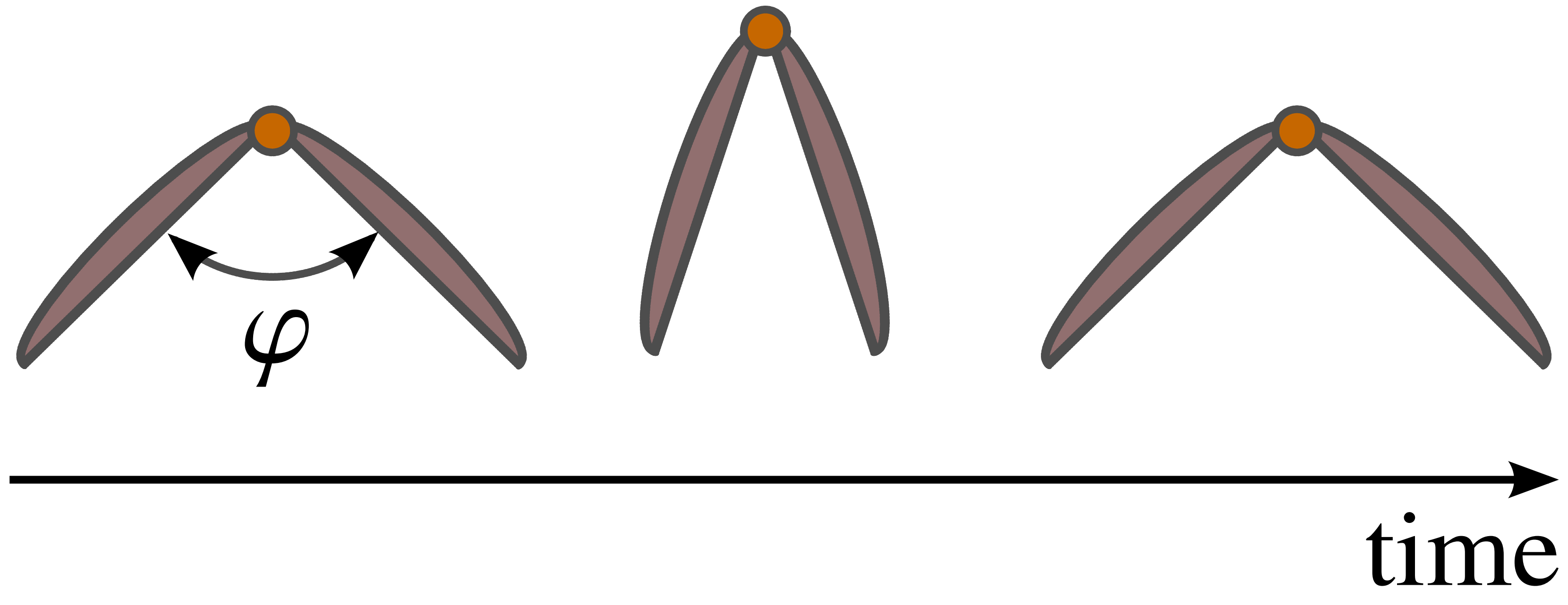


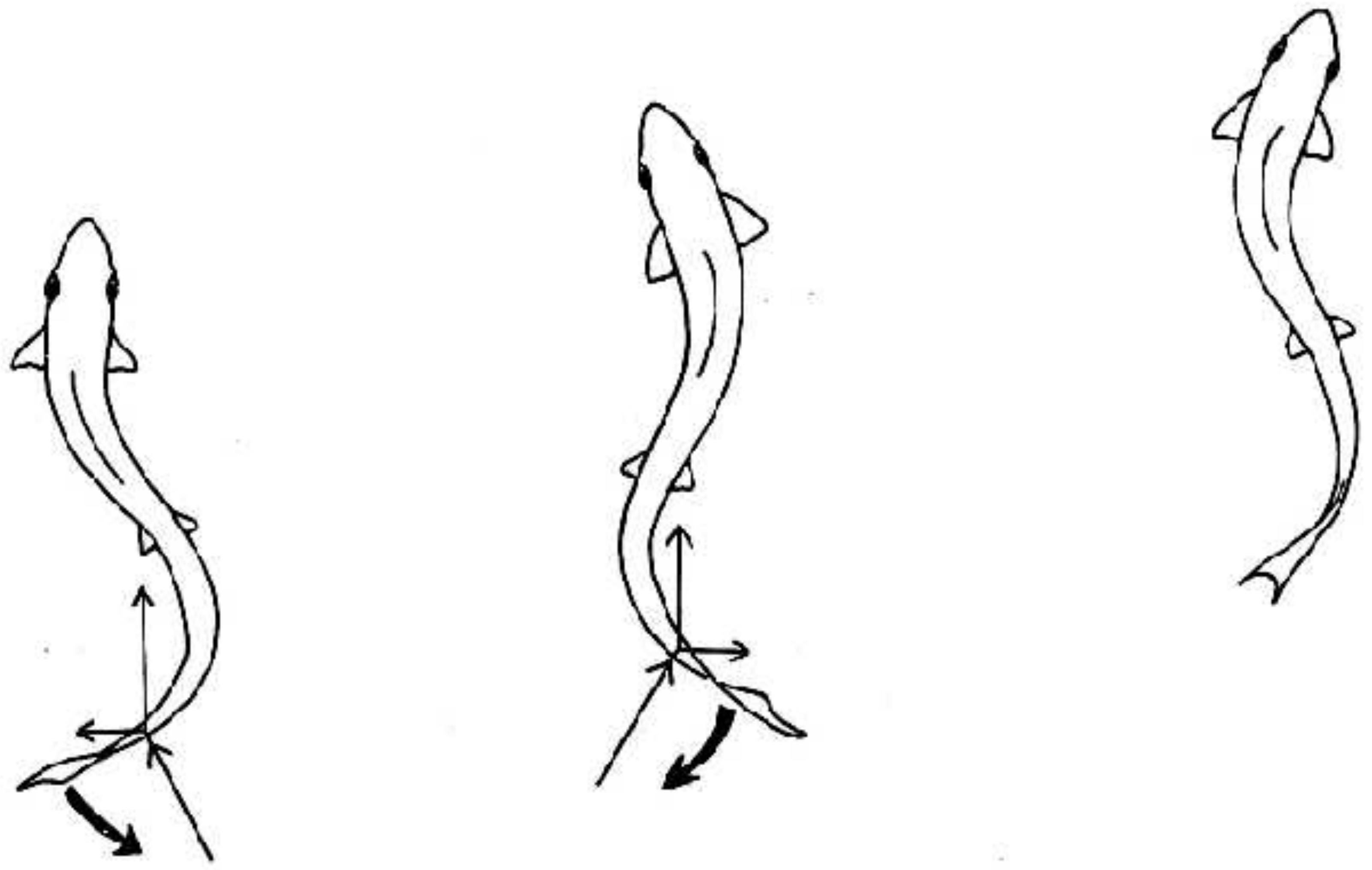
John DeMoss and Kevin Cahill of the Department of Physics & Astronomy. University of New Mexico

Consequences for propulsion and swimming

The Scallop Theorem

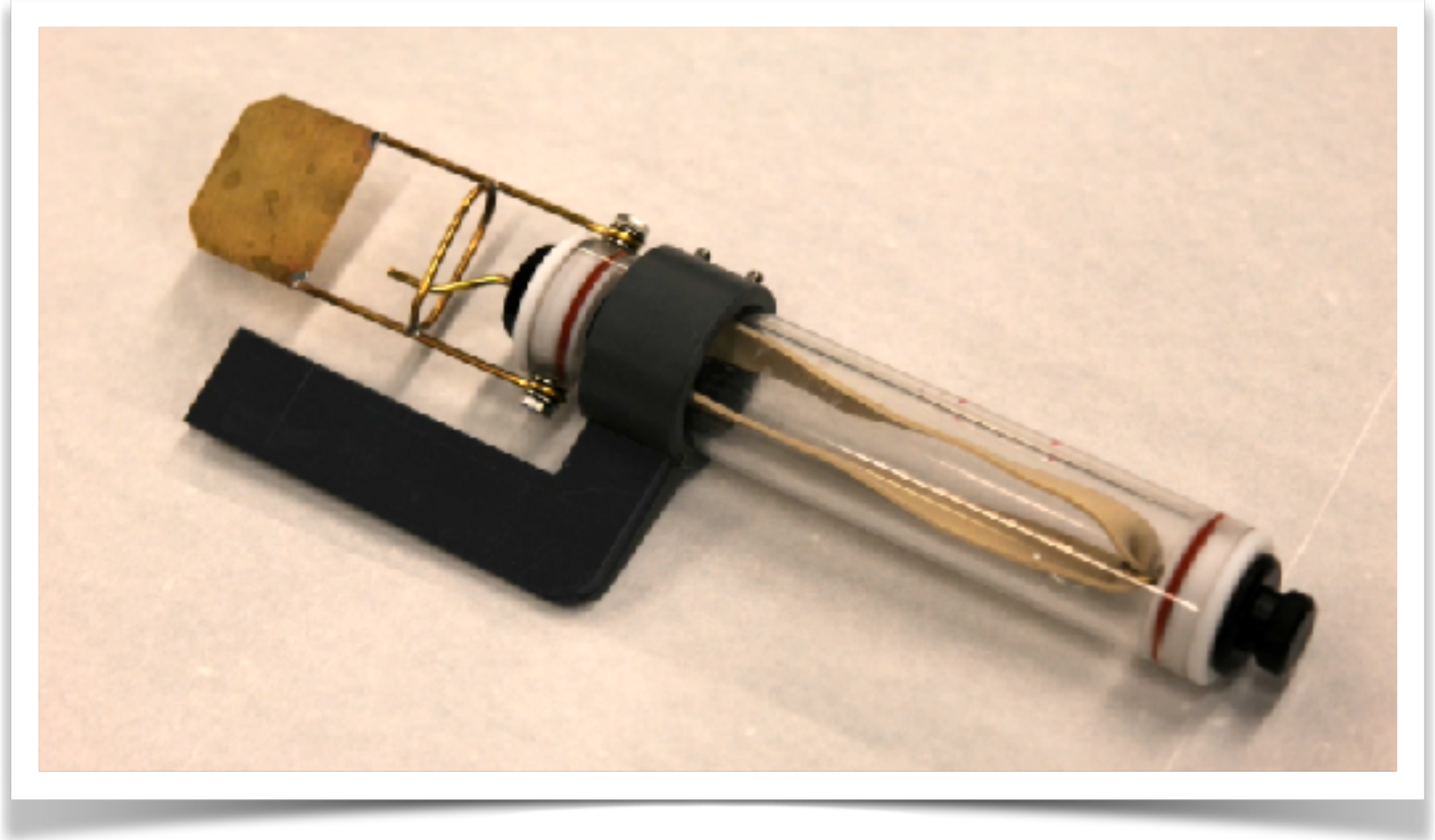
No reversible swimming gait can lead to self-propulsion.



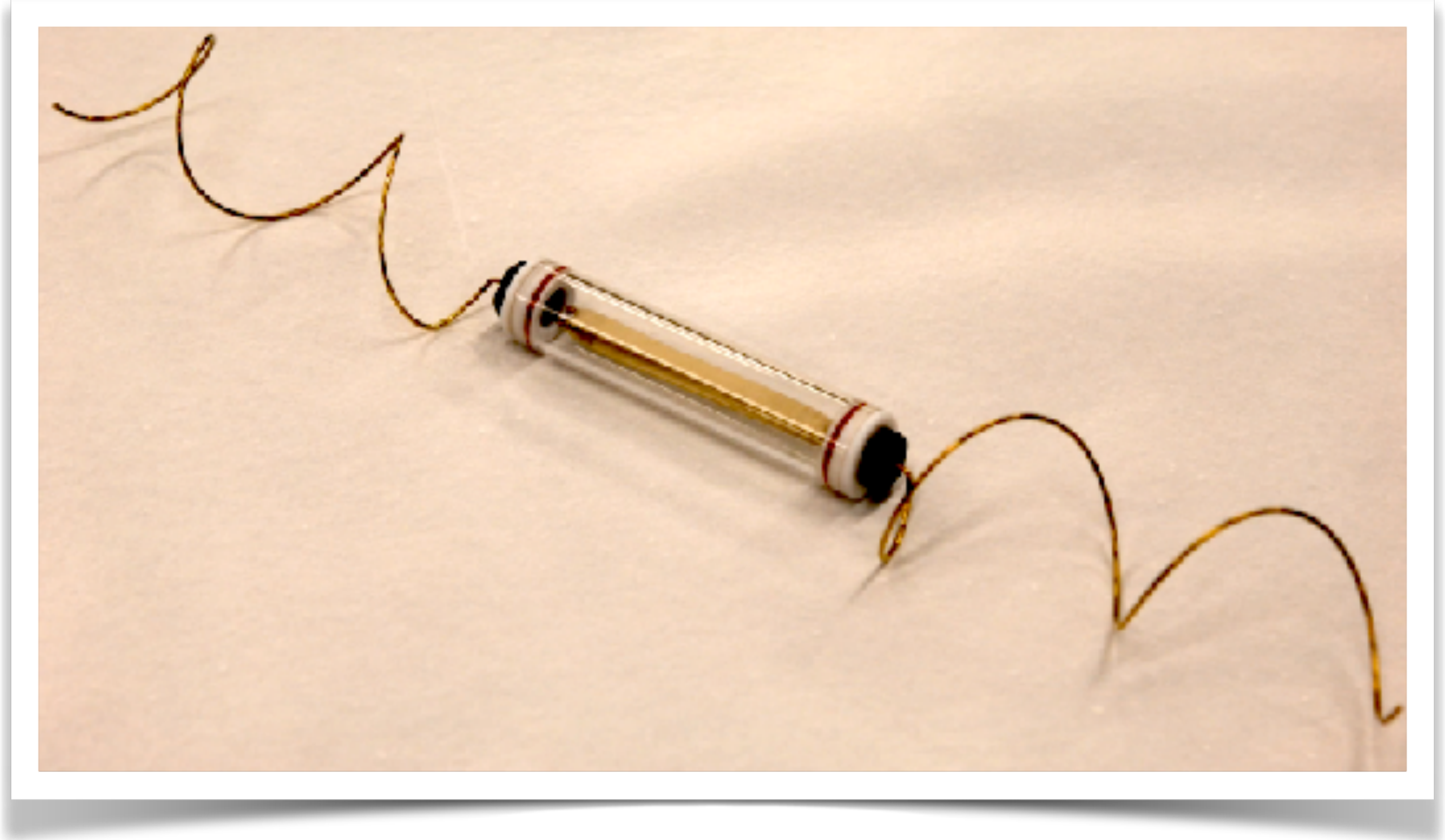


Fish do not swim in honey!

Fish vs. bacteria in viscous fluids



‘Fish’

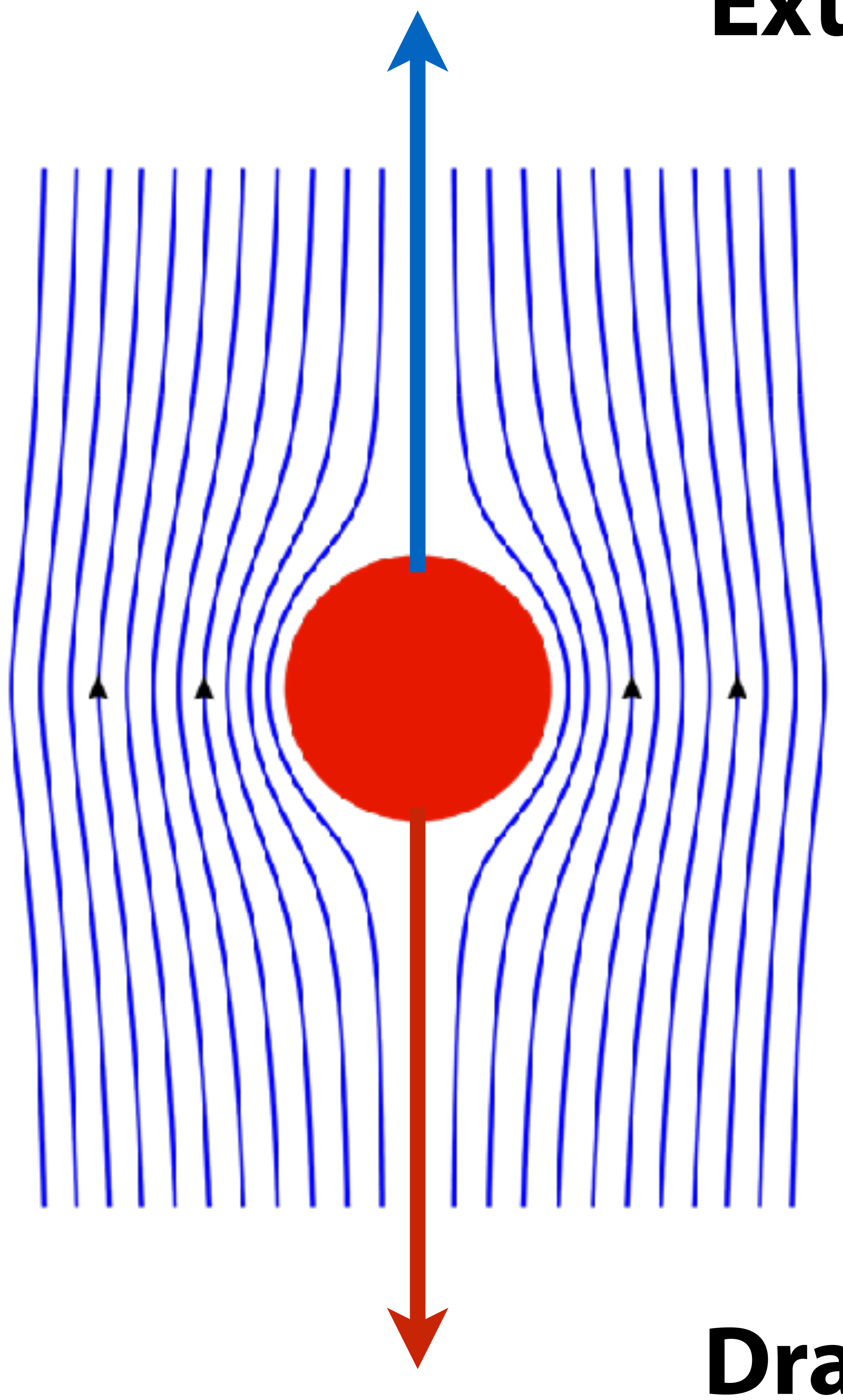


‘Bacterium’

G. I. Taylor (1966) & F. Peaudecerf (2017), University of Cambridge

Stokeslet flow

(Stokeslet) = point force



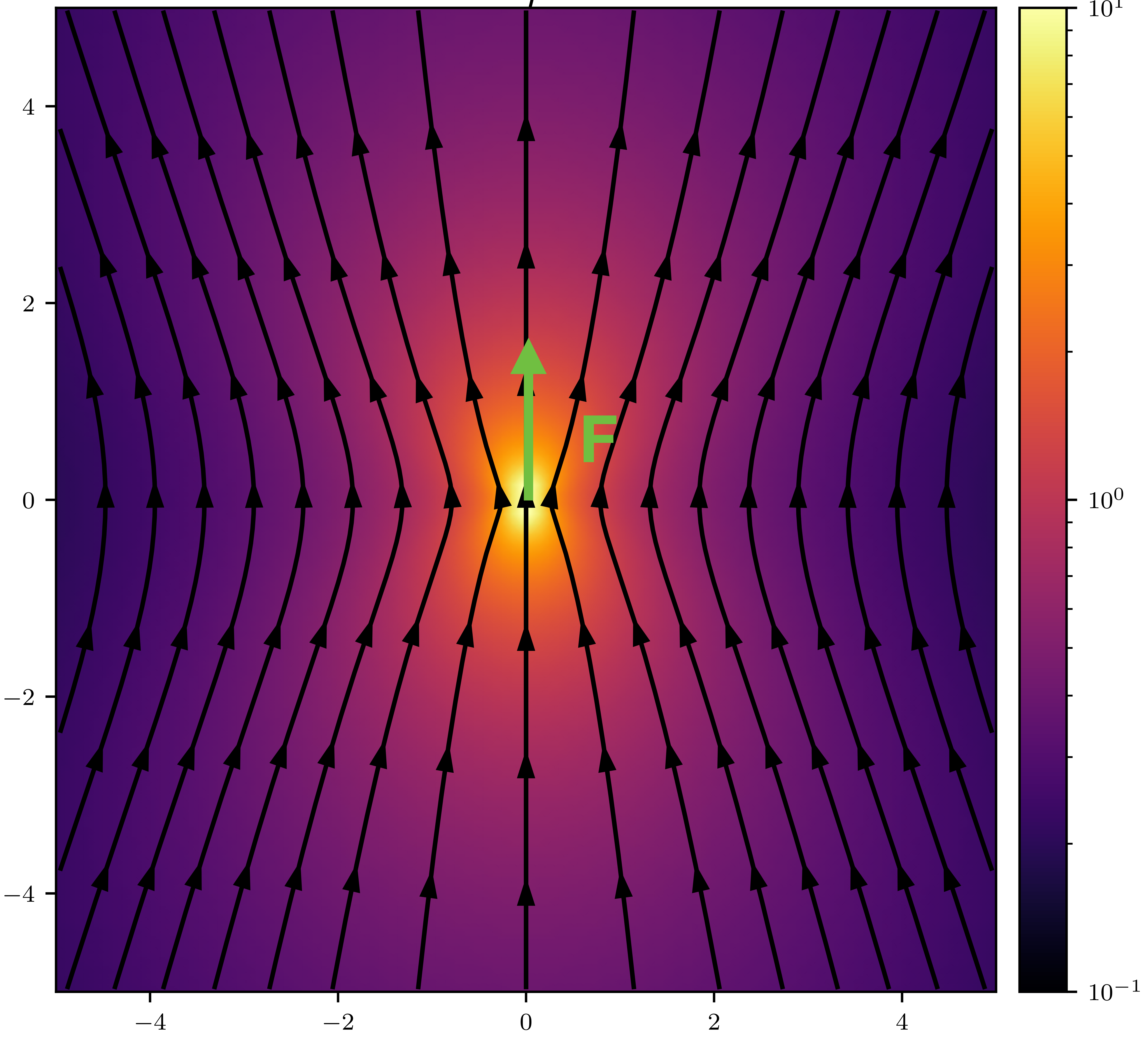
Ext. force F

Drag force

$$\mathbf{F} = -6\pi\eta a\mathbf{V}$$

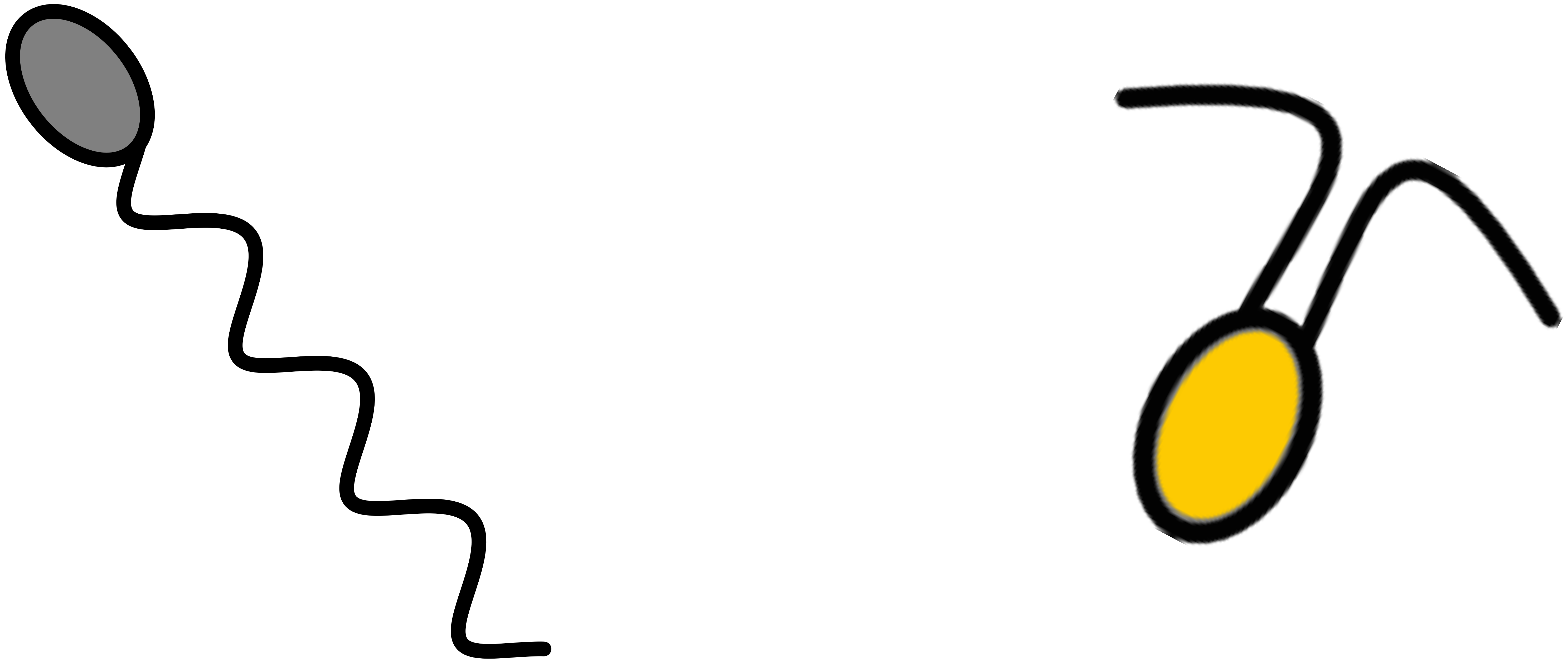
(Stokes law)

$$v(r) = \frac{\mathbf{F}}{8\pi\eta r}(\mathbb{1} + \frac{\mathbf{rr}}{r^2})$$



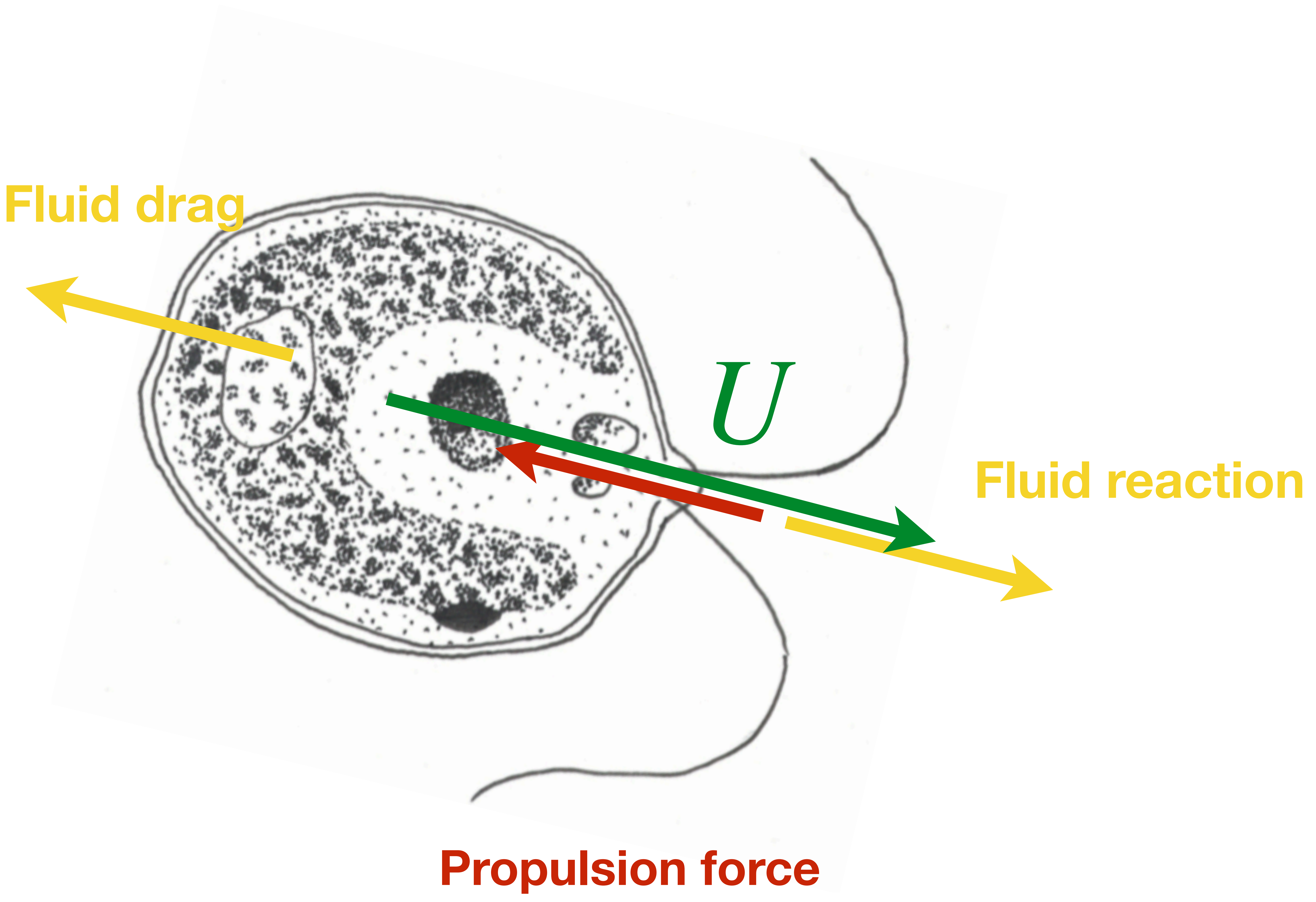
G. Niechwiadowicz

Microscale swimming



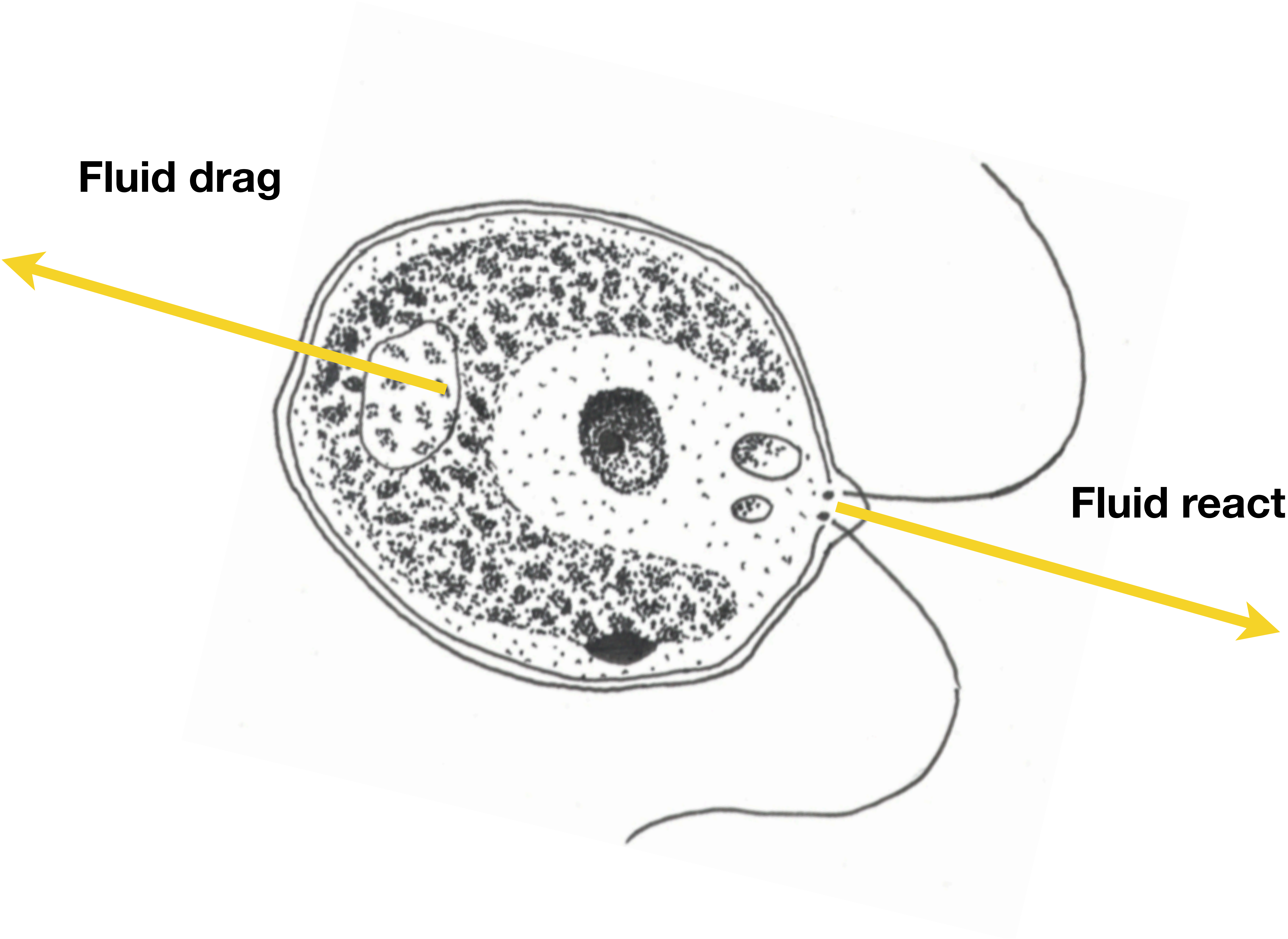
How does the flow field look like?

Forces on a swimmer



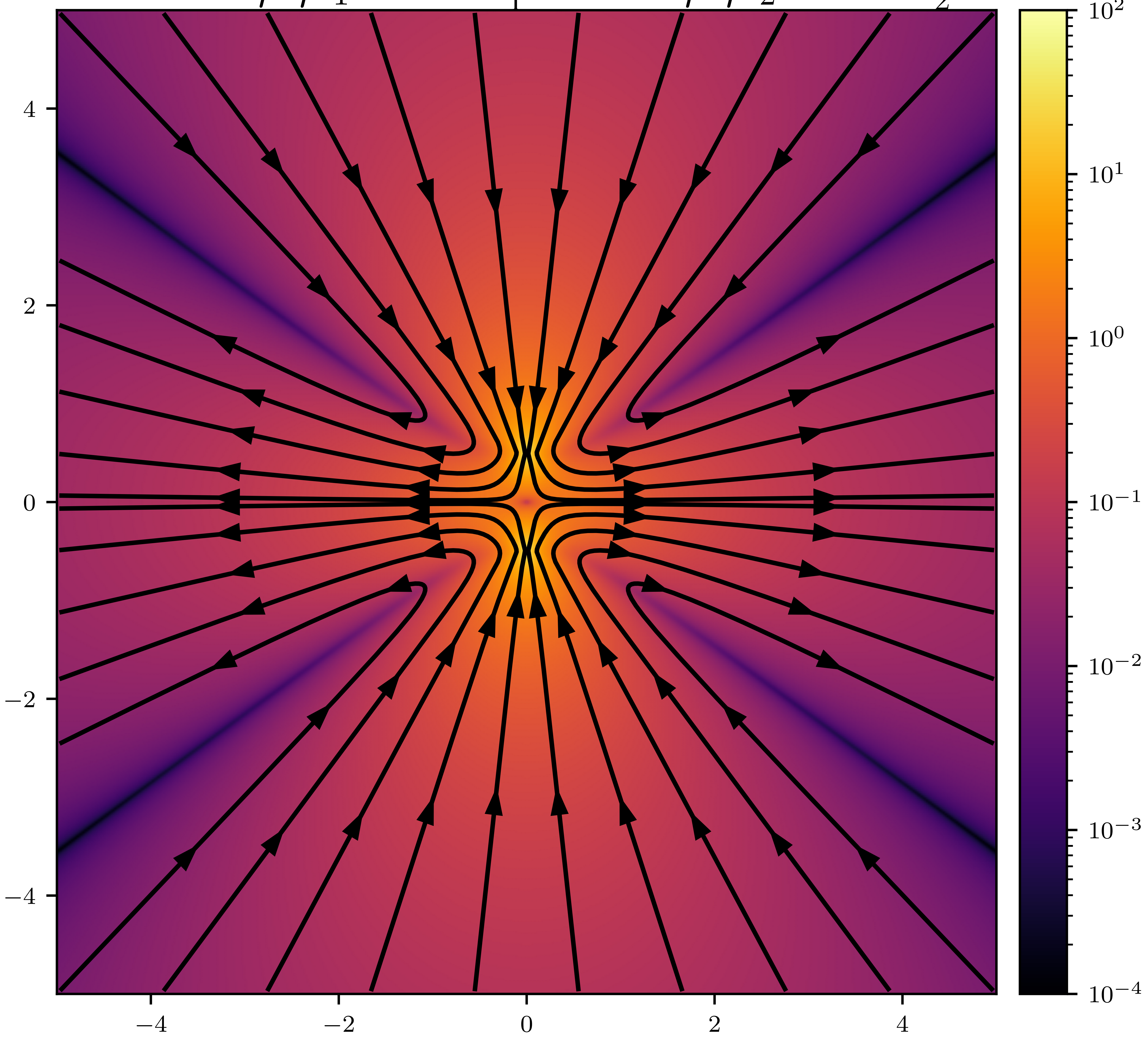
Propulsion force
(on the fluid)

Force dipole



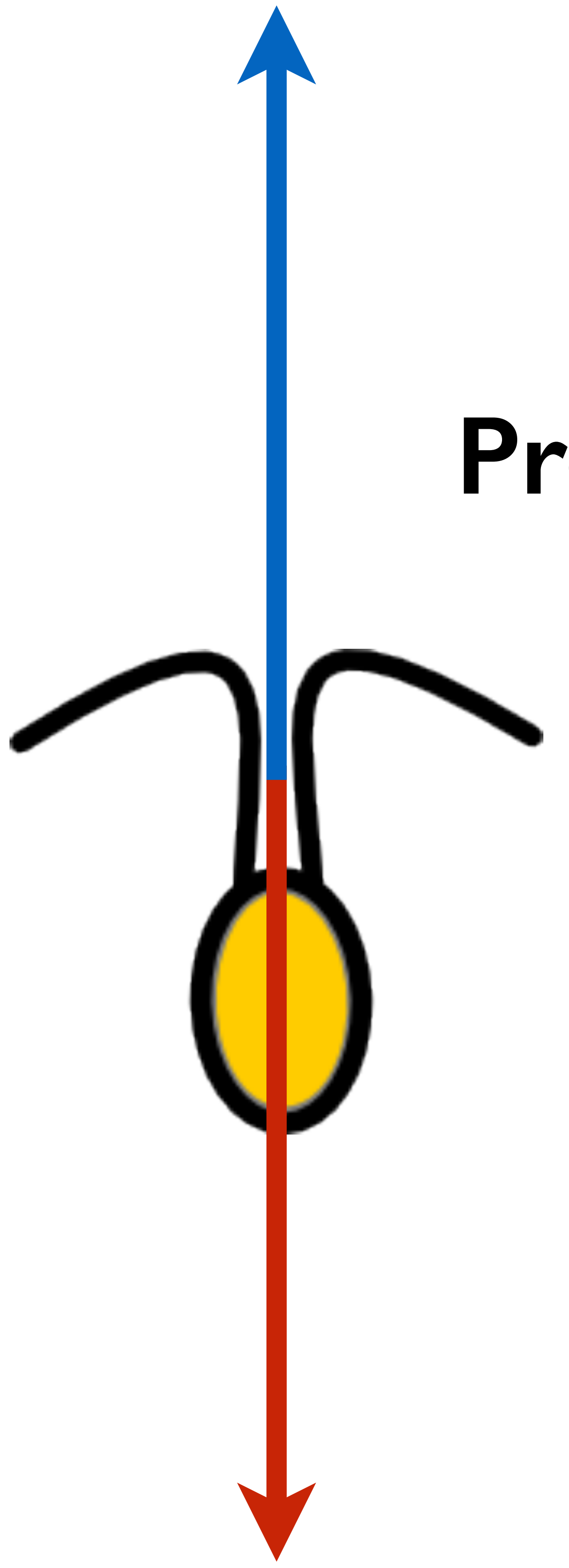
Swimming is force-free!

$$v(r) = \frac{\mathbf{F_1}}{8\pi\mu\eta r_1}\left(\mathbb{1} + \frac{\mathbf{r_1 r_1}}{r_1^2}\right) + \frac{\mathbf{F_2}}{8\pi\mu\eta r_2}\left(\mathbb{1} + \frac{\mathbf{r_2 r_2}}{r_2^2}\right)$$



G. Niechwiadowicz

Dipolar flow

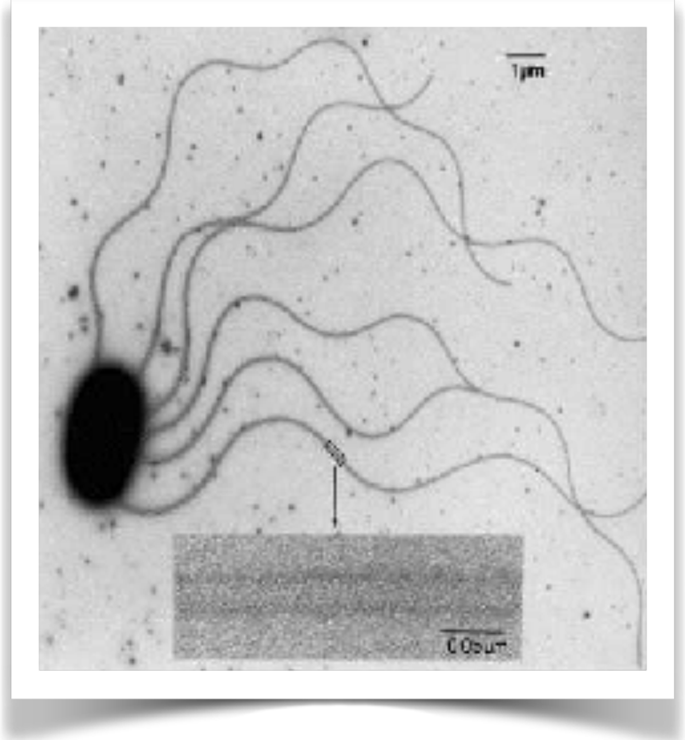


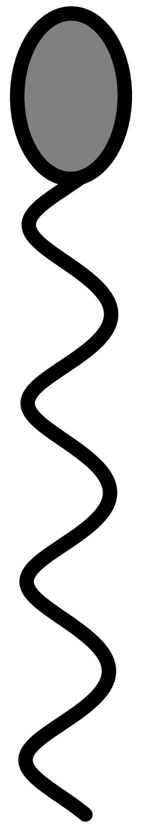
Propulsion

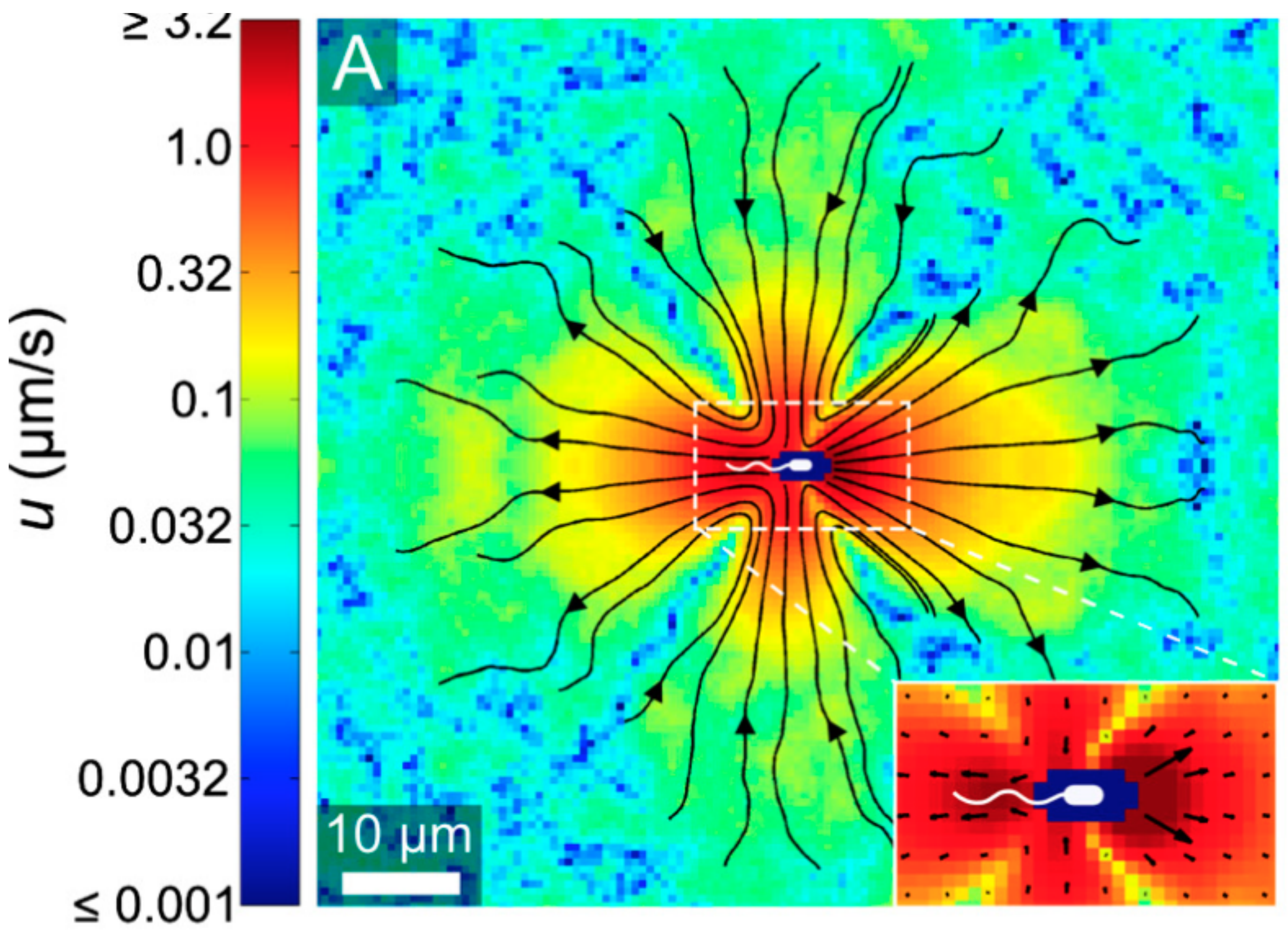
Drag

Flow around swimming microorganisms

Swimming bacterium *E. coli*

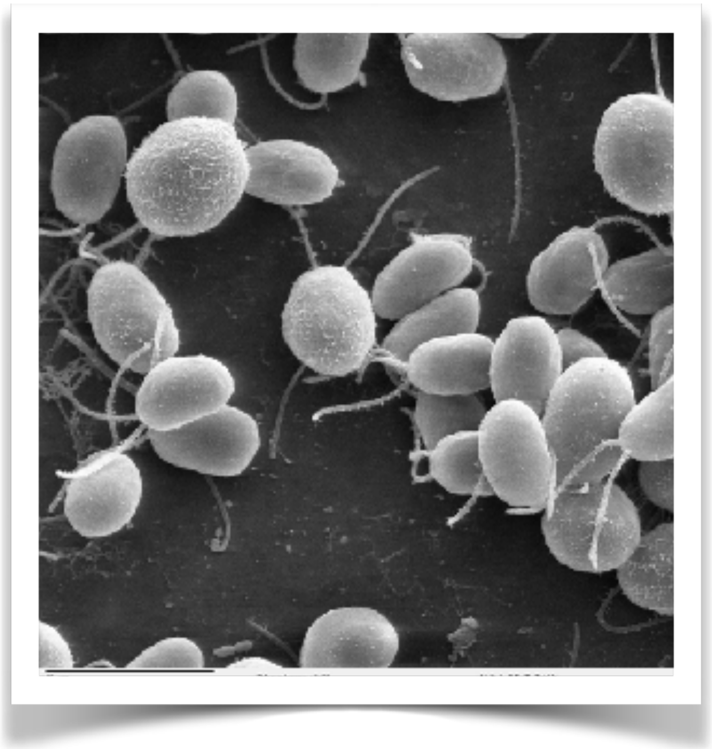


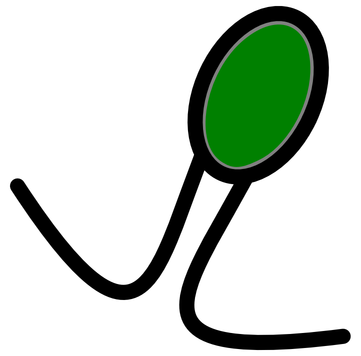


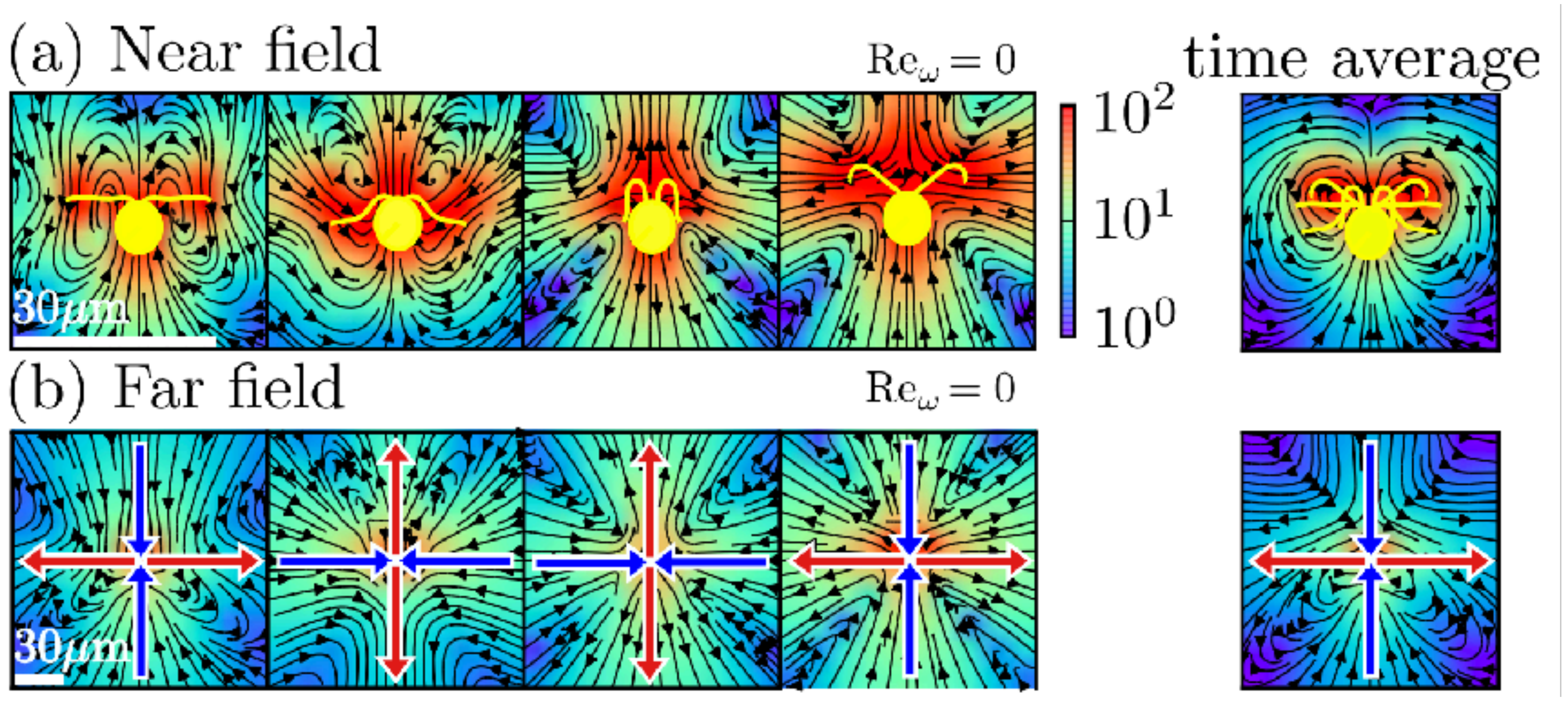


Drescher et al. (2011)

Swimming alga *C. reinhardtii*

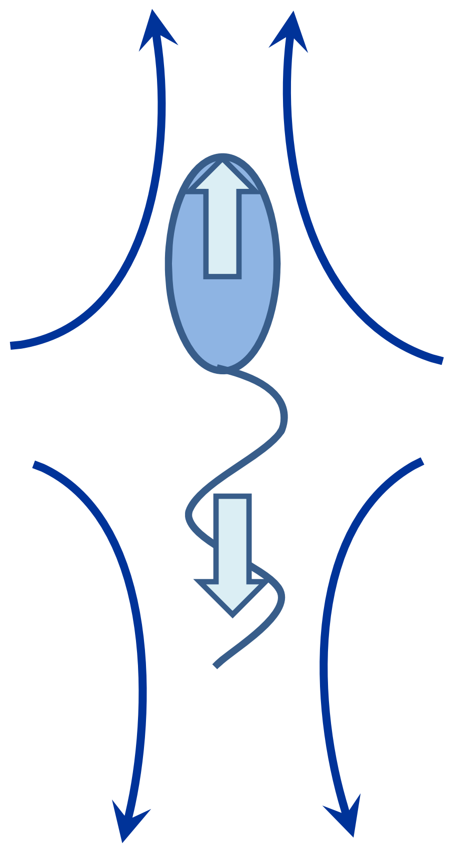






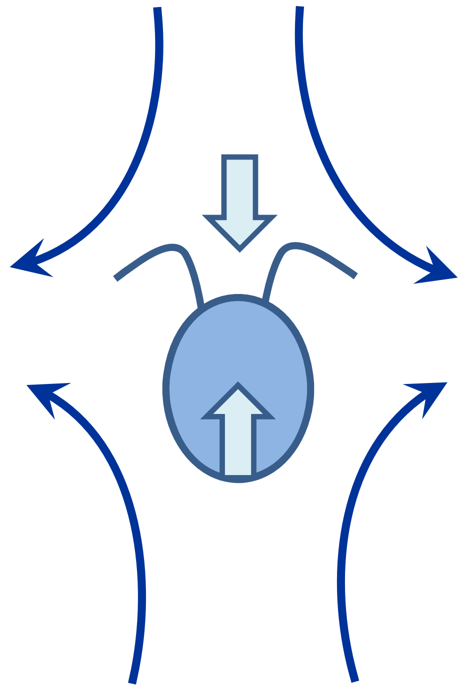
Klindt & Friedrich (2015)

Generic flow field

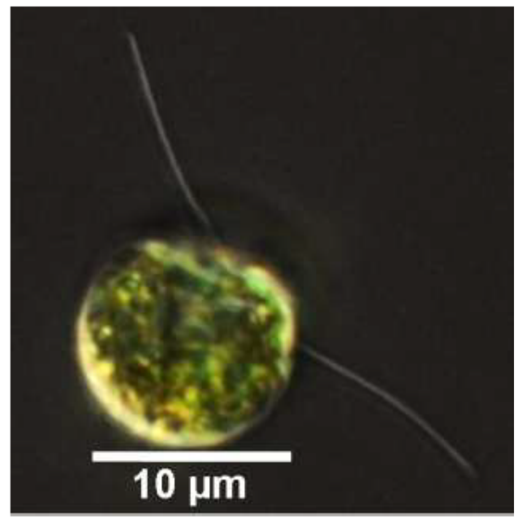


Pusher: $p > 0$

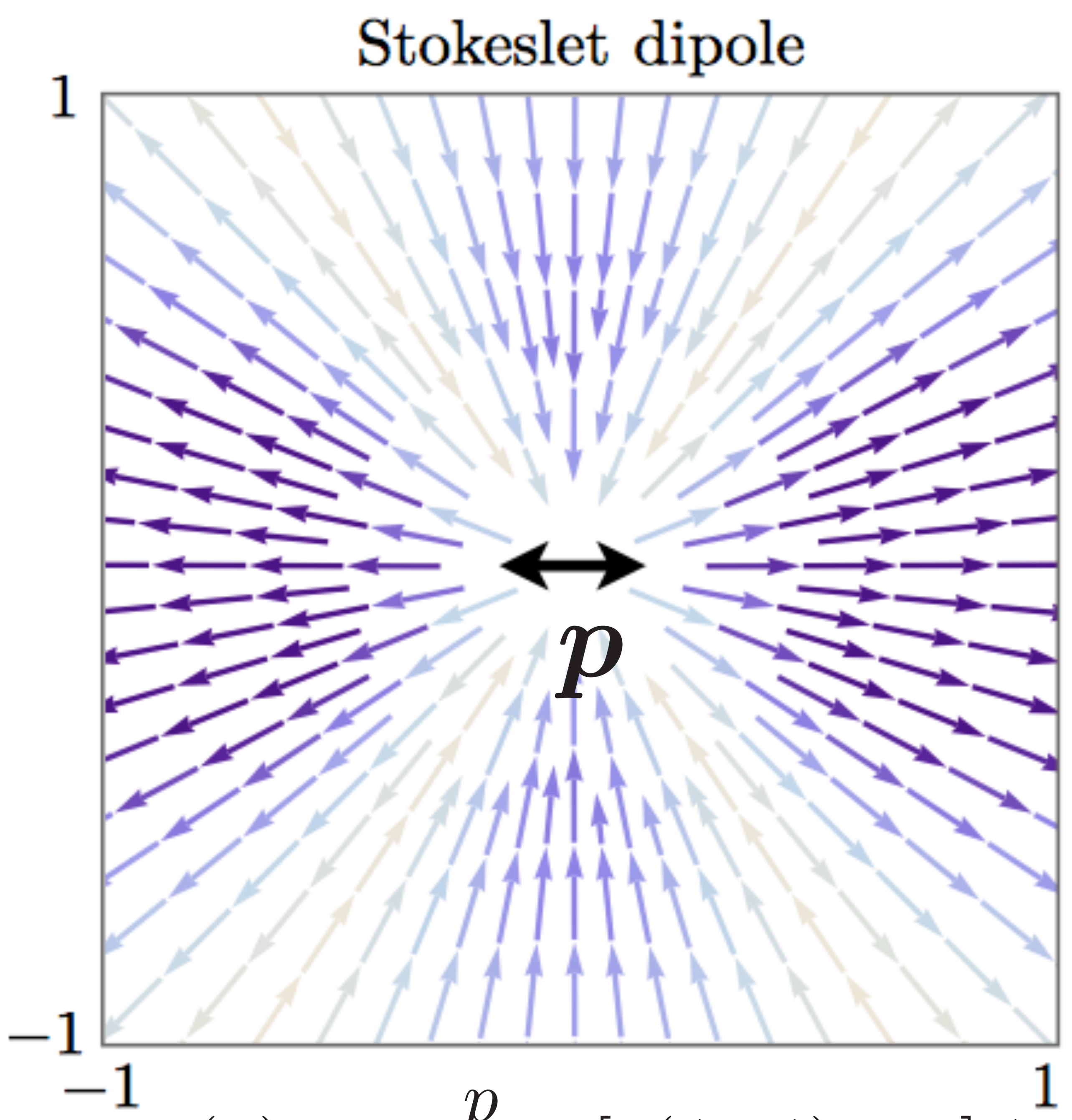
E. coli



Puller: $p < 0$



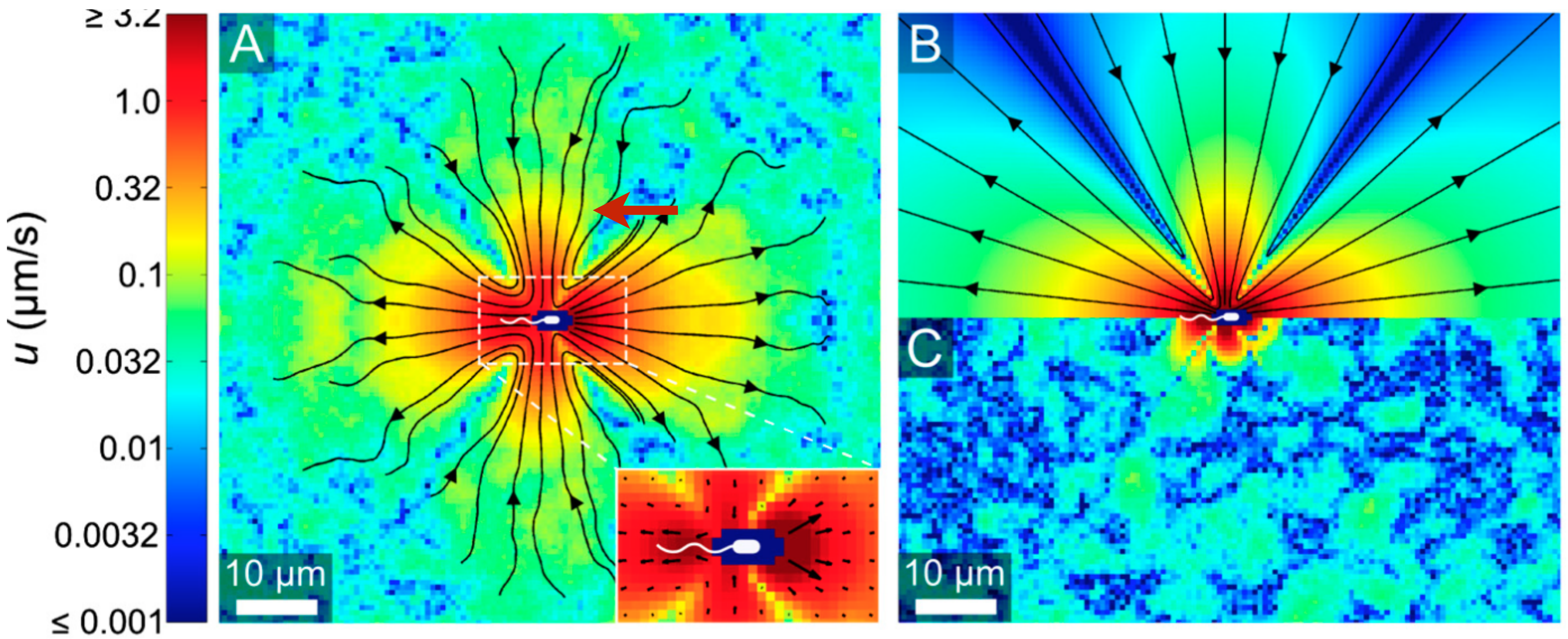
C. reinhardtii



$$\boldsymbol{v}(\boldsymbol{r}) = \frac{p}{8\pi\eta r^2}\left[3(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}) - 1\right]\hat{\boldsymbol{r}}$$

Generic far-field behaviour of the flow field around a force-free object – **dipolar flow**

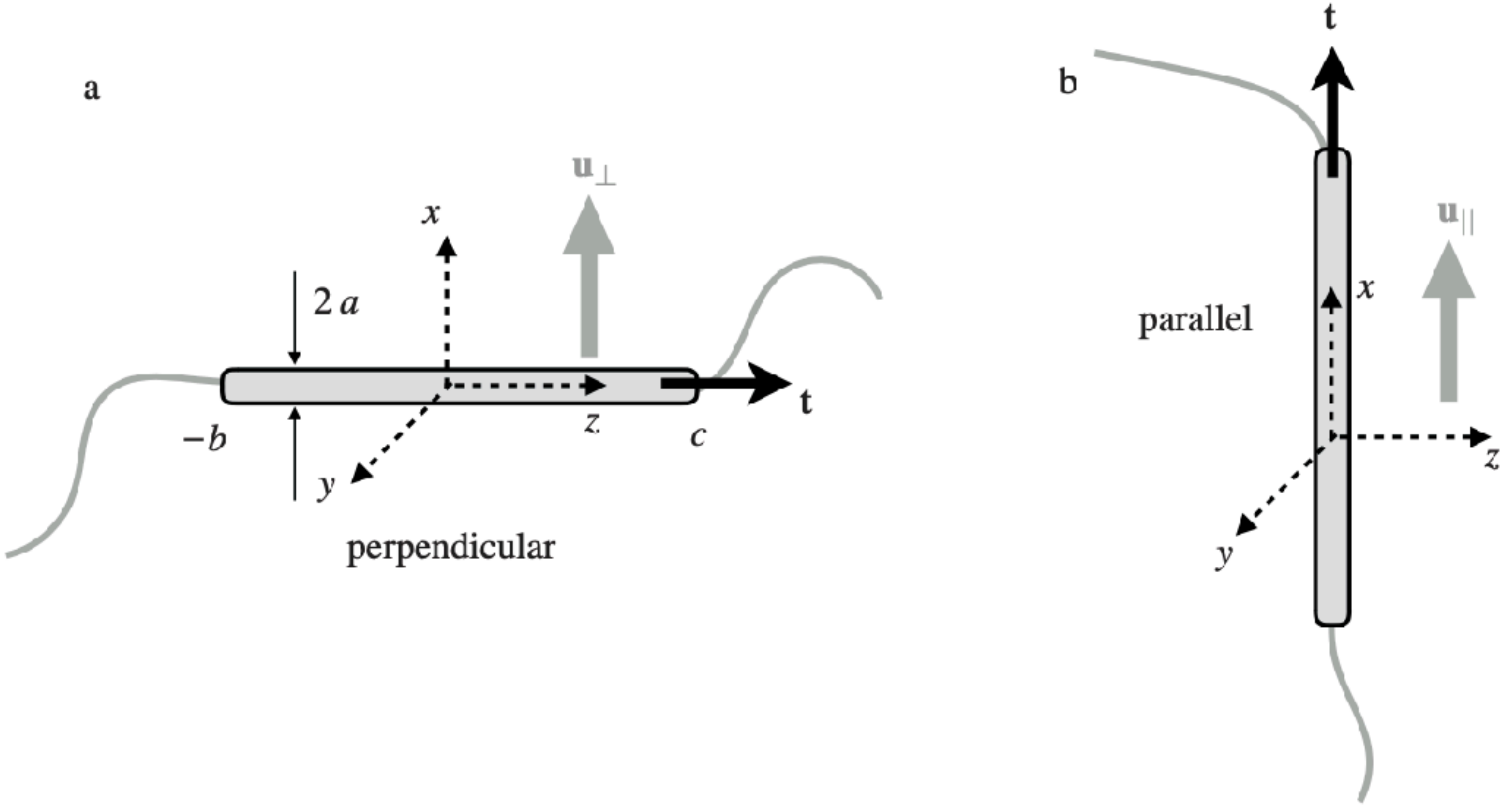
Universal features of microscale flows



full flow field

dipolar term subtracted

Slender filament in flow



Lauga (2020)

$$\boldsymbol{U}(s) = -\left[\alpha \hat{\boldsymbol{t}}\hat{\boldsymbol{t}} + \beta(\mathbf{1} - \hat{\boldsymbol{t}}\hat{\boldsymbol{t}})\right] \cdot \boldsymbol{f}(s)$$

Resistive force theory (RFT)

(local relationship)

Gray & Hancock (1955)

☞ **Slender body theory**

Elastohydrodynamics of thin filaments

Hydrodynamic forces

Fluid friction

Hydrodynamic interactions

Elastic forces

Bending

Twisting

Active deformation

Other

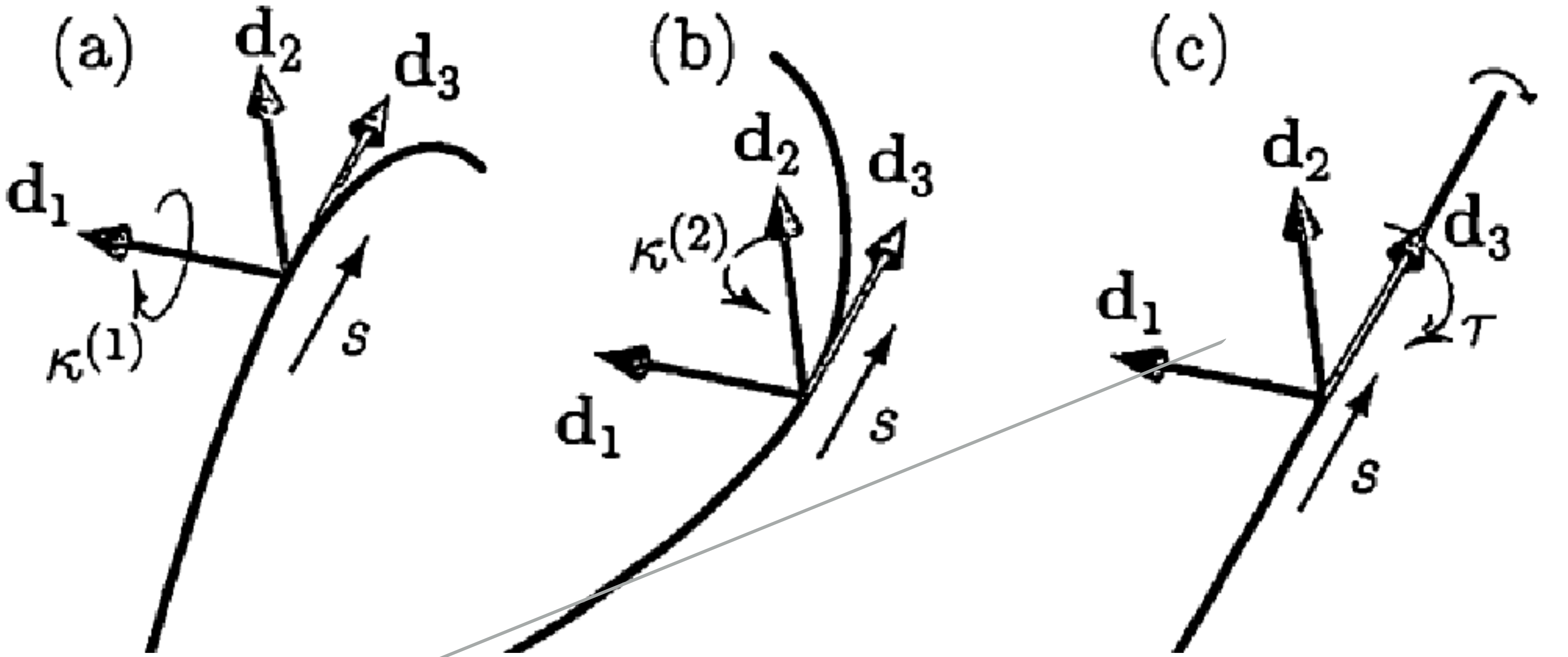
Steric, electrostatic, etc.

Elastic energy of a filament

Deformations cost energy!

Local modes of deformation:

two curvatures (a), (b)   **torsion (twist) (c)**

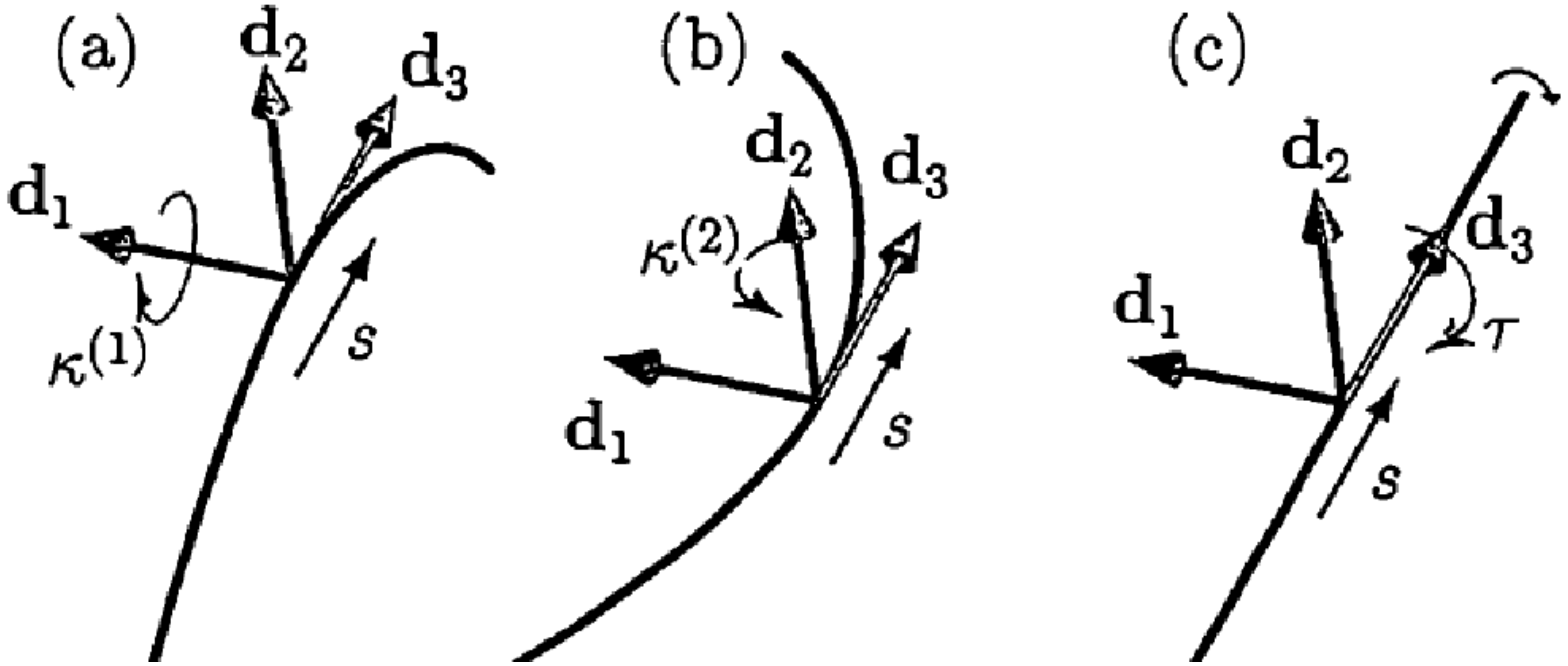


+ compressional stresses

Audoly & Pomeau

Fully analogous to a spring: $F = kx$ $\mathcal{E} = \frac{k}{2}x^2$

Elastic energy of a filament



$$\mathcal{E}_{\mathrm{rod}} = \underbrace{\int \mathrm{d}s \left(\frac{EI_1}{2} (\kappa_1(s))^2 + \frac{EI_2}{2} (\kappa_2(s))^2 + \frac{SJ}{2} (\tau(s))^2 \right)} + \underbrace{\int \mathrm{d}s \sigma(s)}$$

Material properties:

Young's modulus *E*

Shear modulus *S*

Moment of inertia *I*

Moment of twist *J*

Shape properties:

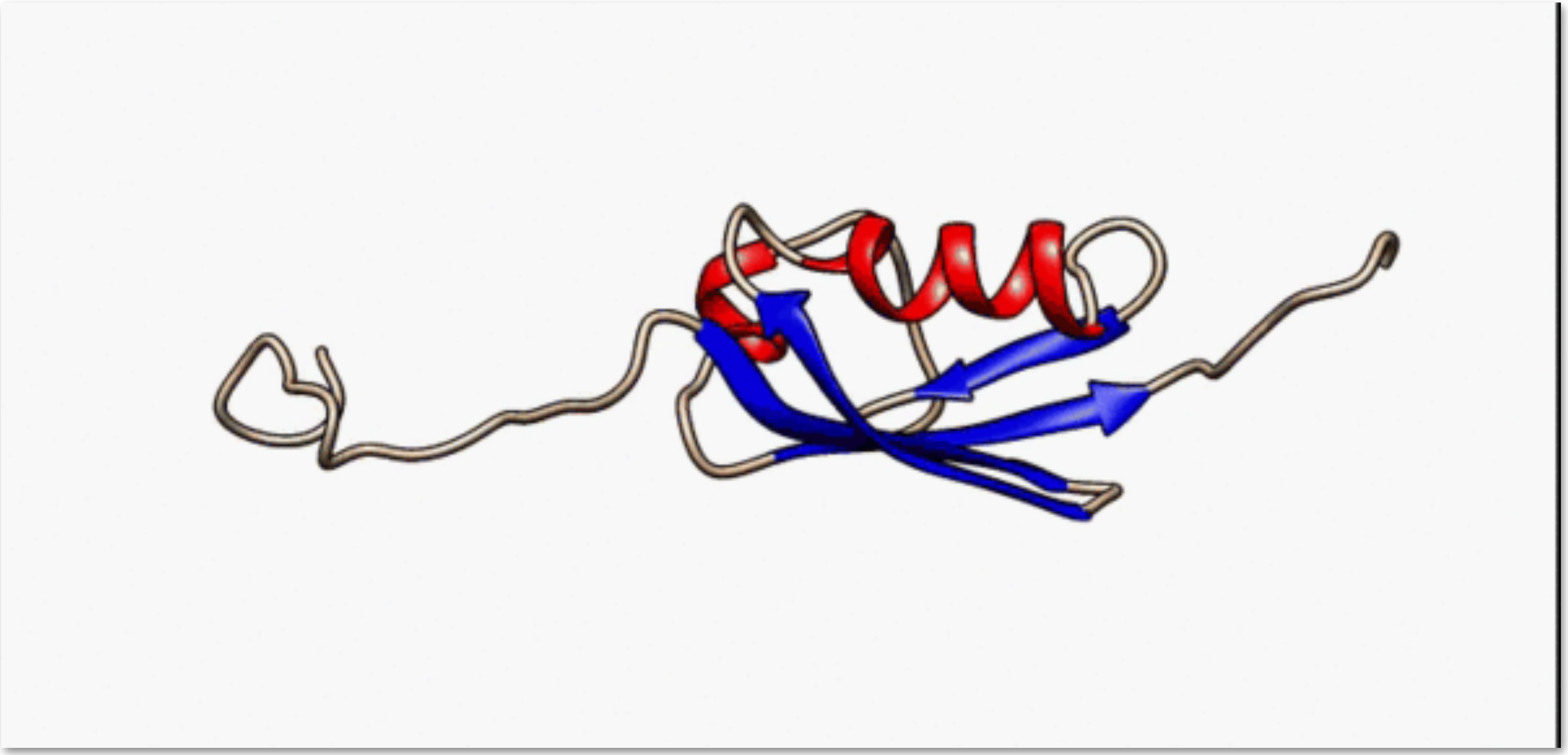
Curvature $\kappa_{1,2}(s)$

Torsion $\tau(s)$

$\sigma(s)$ Internal tension

Fully analogous to a spring: $F = kx$ $\mathcal{E} = \frac{k}{2} x^2$

Elastohydrodynamics of biomacromolecules

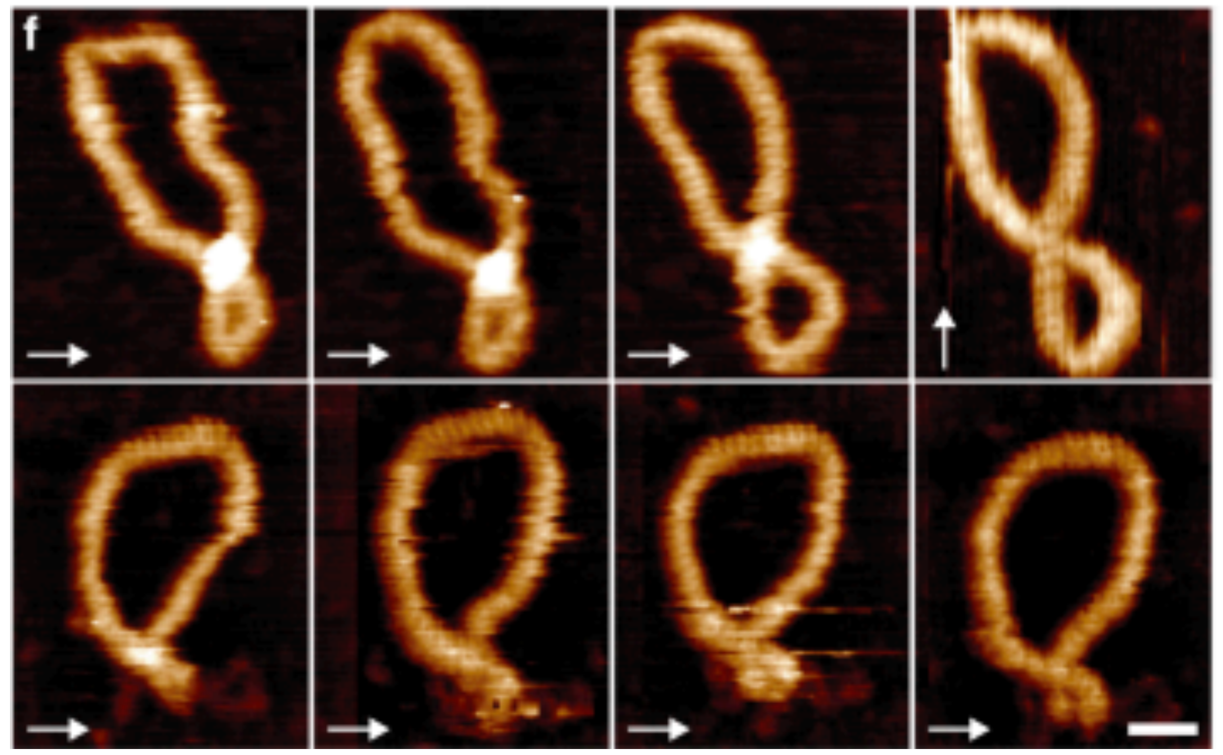


Interplay of: hydrodynamics, elasticity, electrostatics, steric, thermal

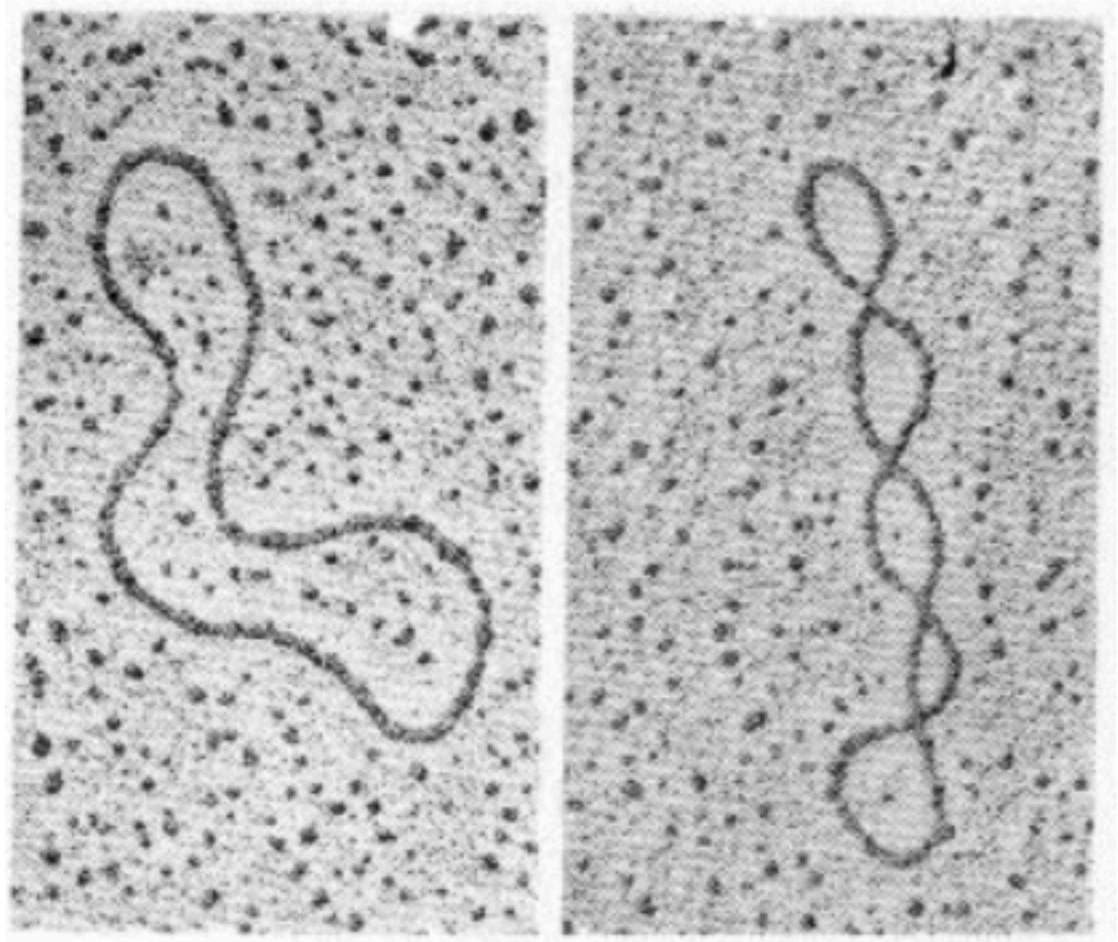
Key quantity: **persistence length** $L_p \sim \dfrac{B}{k_B T}$

elastic
vs.
thermal

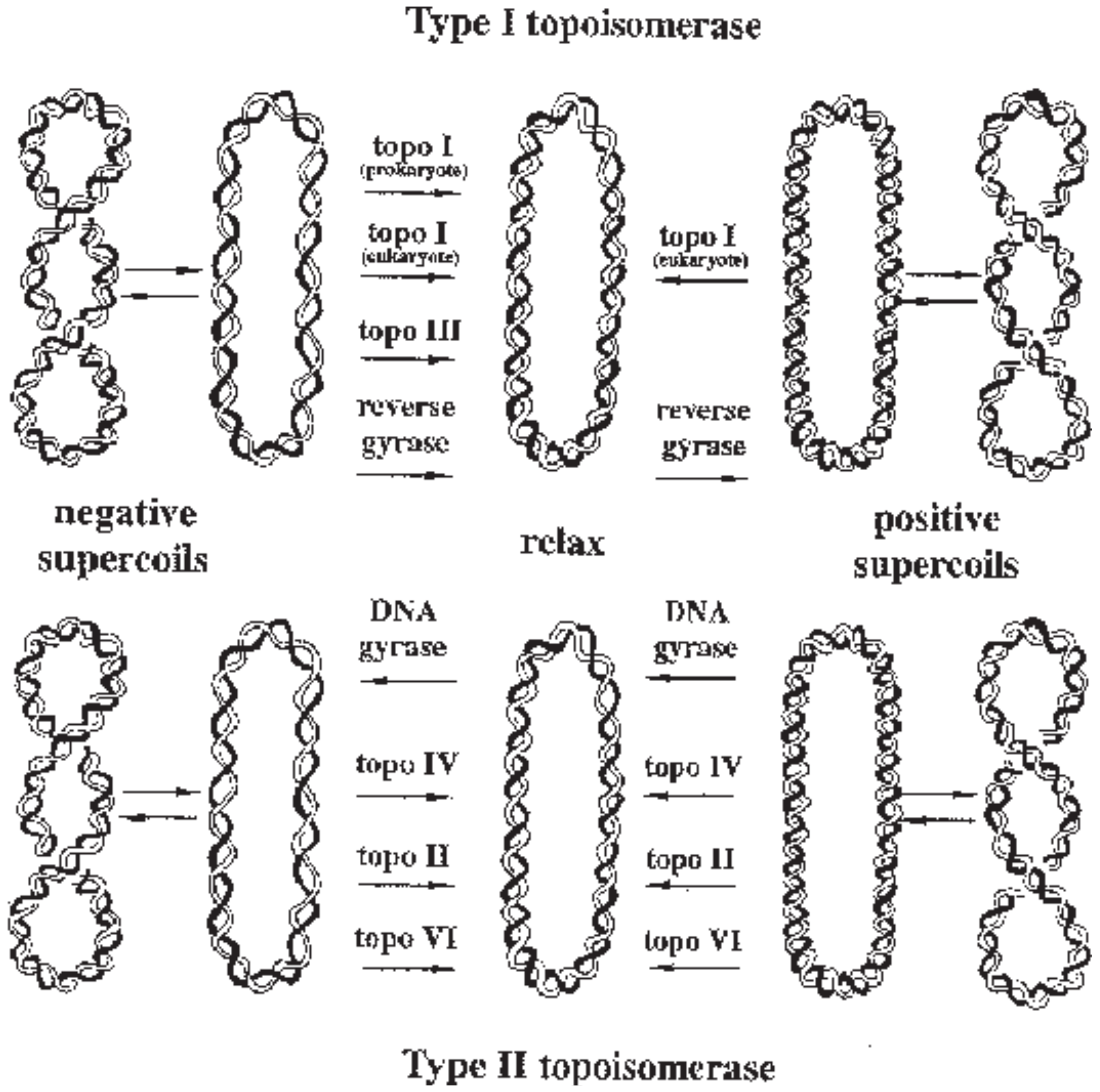
DNA supercoiling



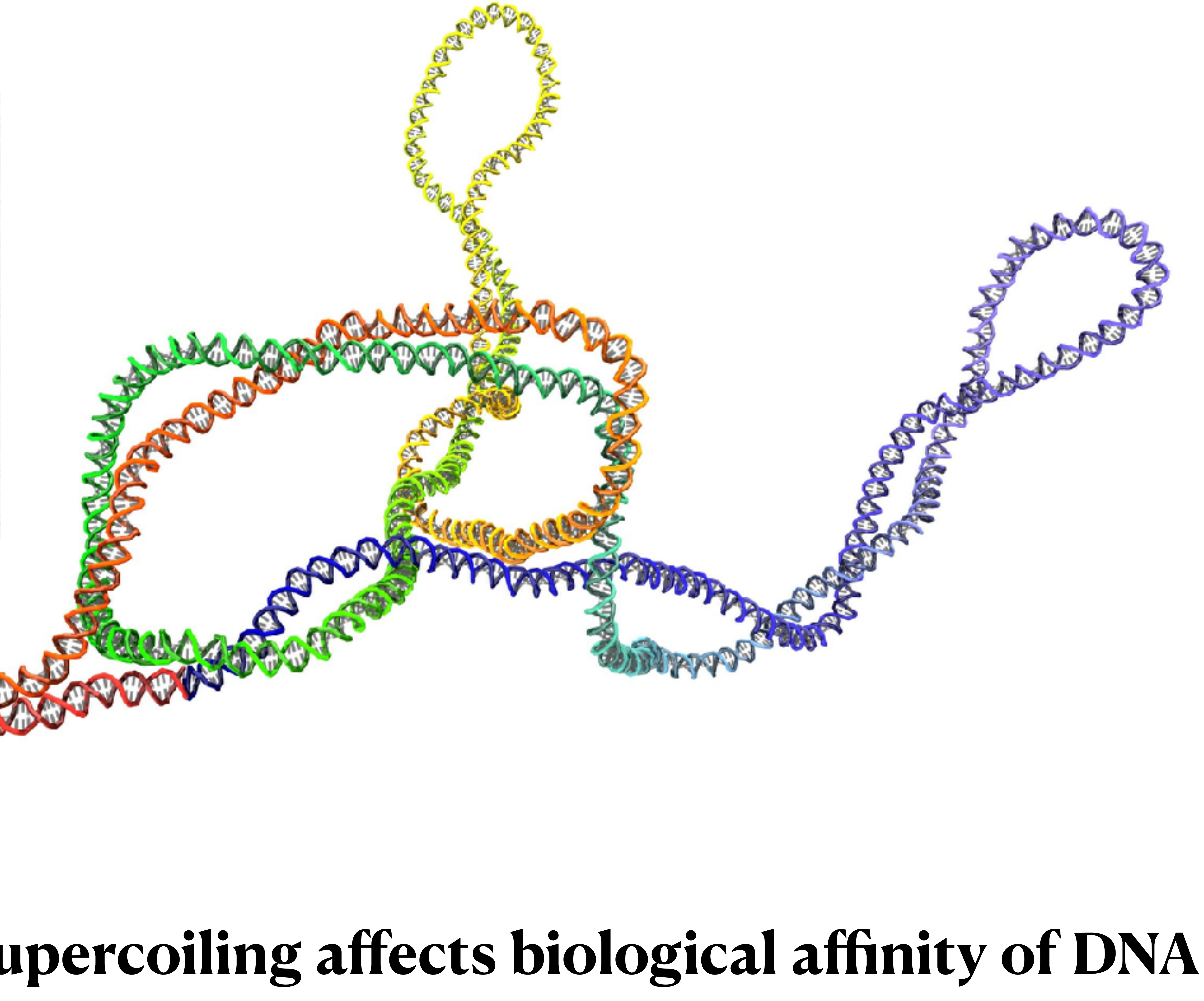
Pyne et al, *Nat. Commun,* (2021).



Boles et al, *J. Mol. Biol.* (1990).



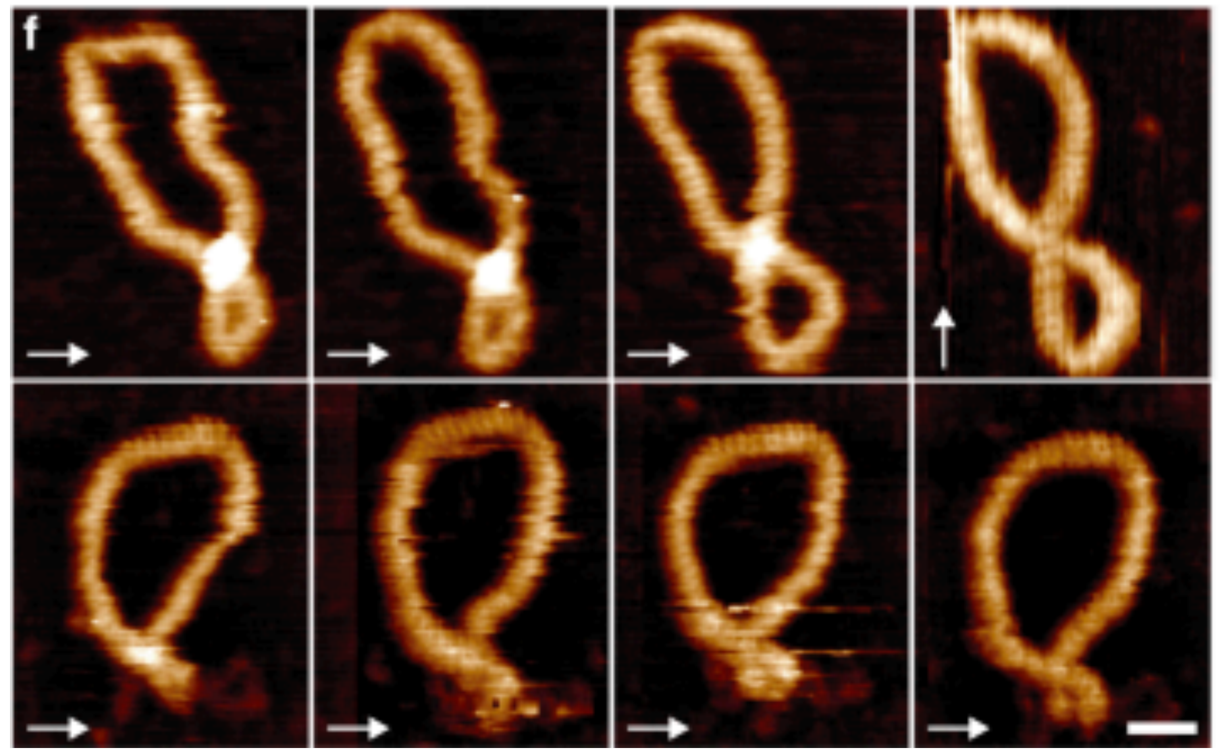
Kato & Kikuchi, Nagoya J. Med. Sci. (1998)



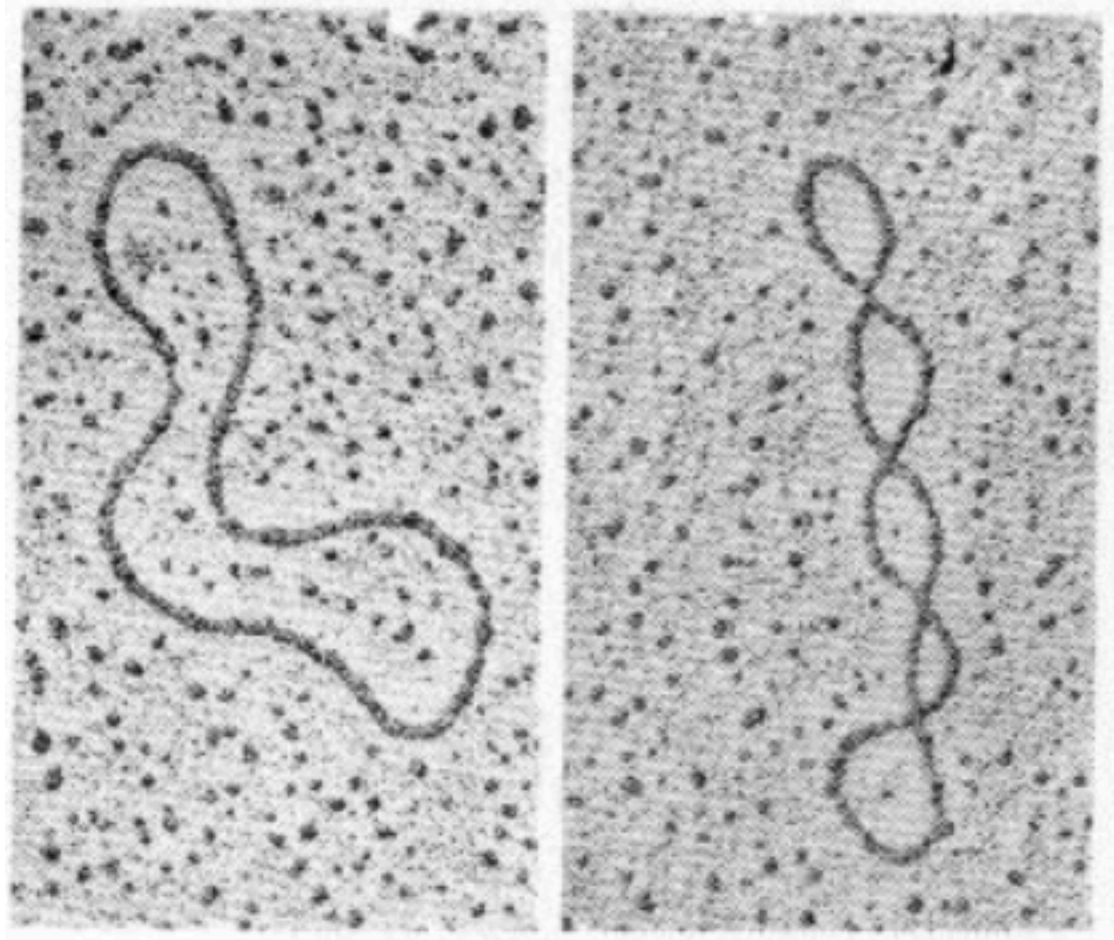
Supercoiling affects biological affinity of DNA

Biology ⇔ Topology ⇔ Physics

Static picture – energy minimization



Pyne et al, *Nat. Commun*, (2021).



Boles et al, *J. Mol. Biol.* (1990).

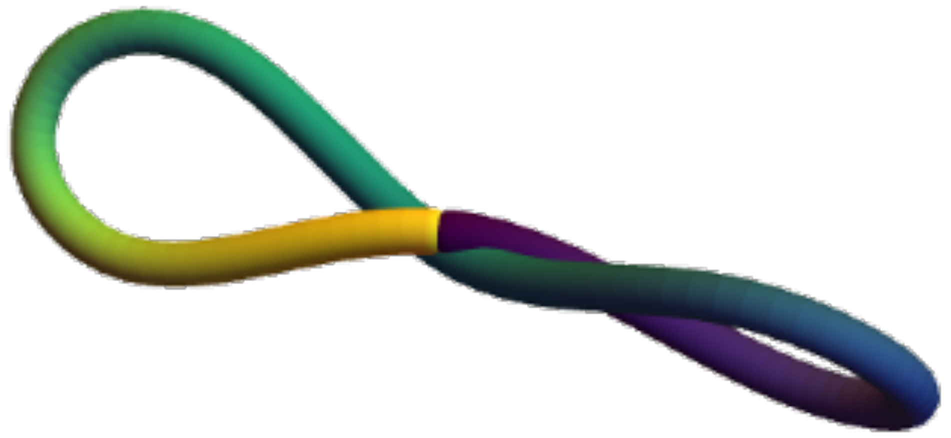
DNA minicircles

L ~ 30 nm

L ~ 336 bp

L_p ~ 50 nm

very stiff molecules



Bending + twisting
elastic energy

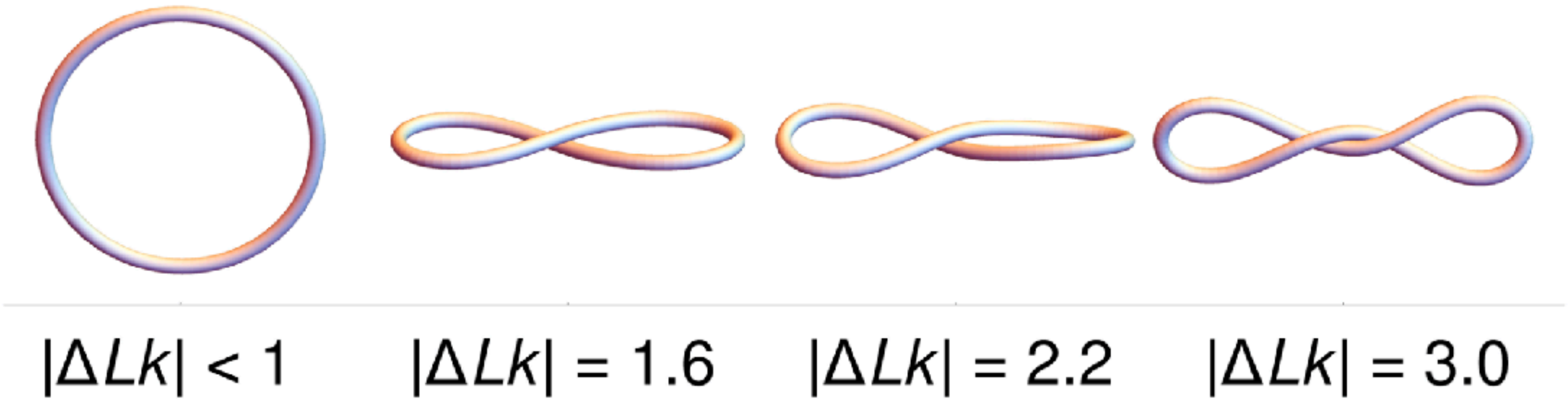
$$E_{\mathrm{rod}} = \frac{1}{2}\int A\left(\kappa^2 + \omega\Omega^2\right)\mathrm{d}s$$

Twist ⇋ Writhe

$$Lk = Tw + Wr$$

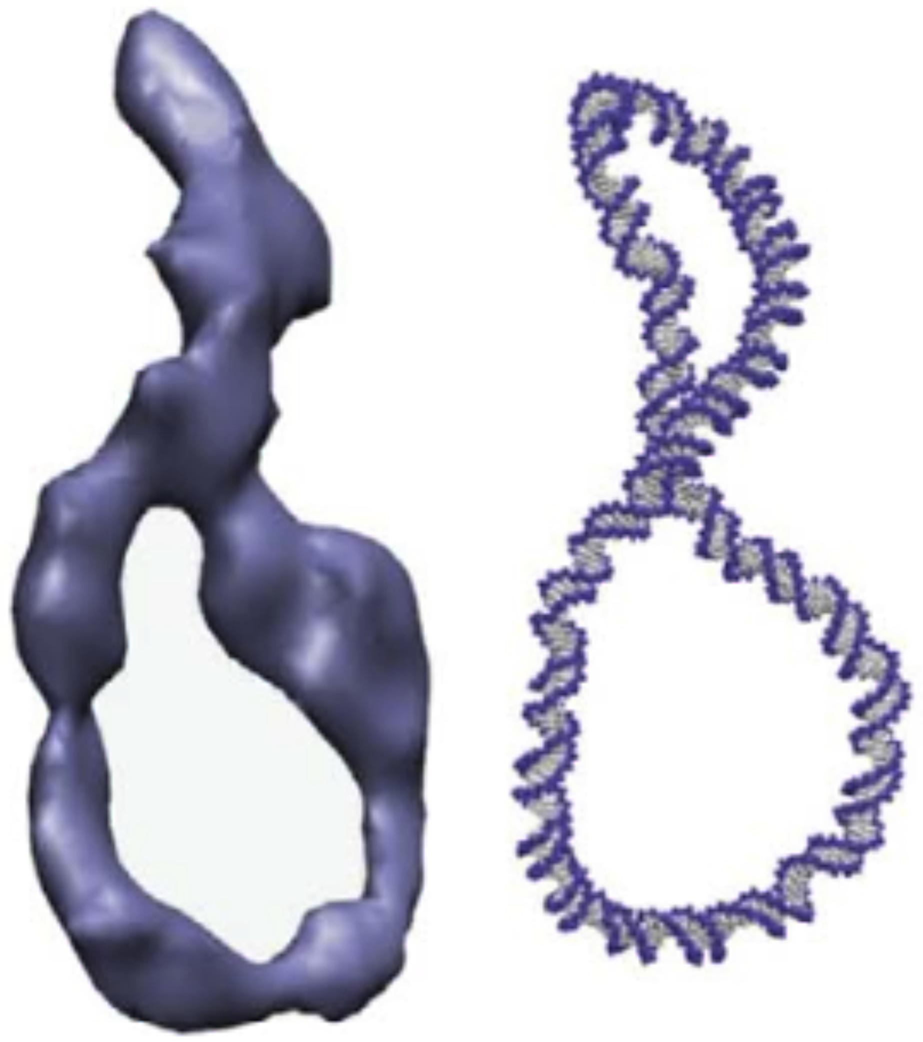
Waszkiewicz et al., Nucl. Acids Res. (2023)

Shapes of DNA minicircles

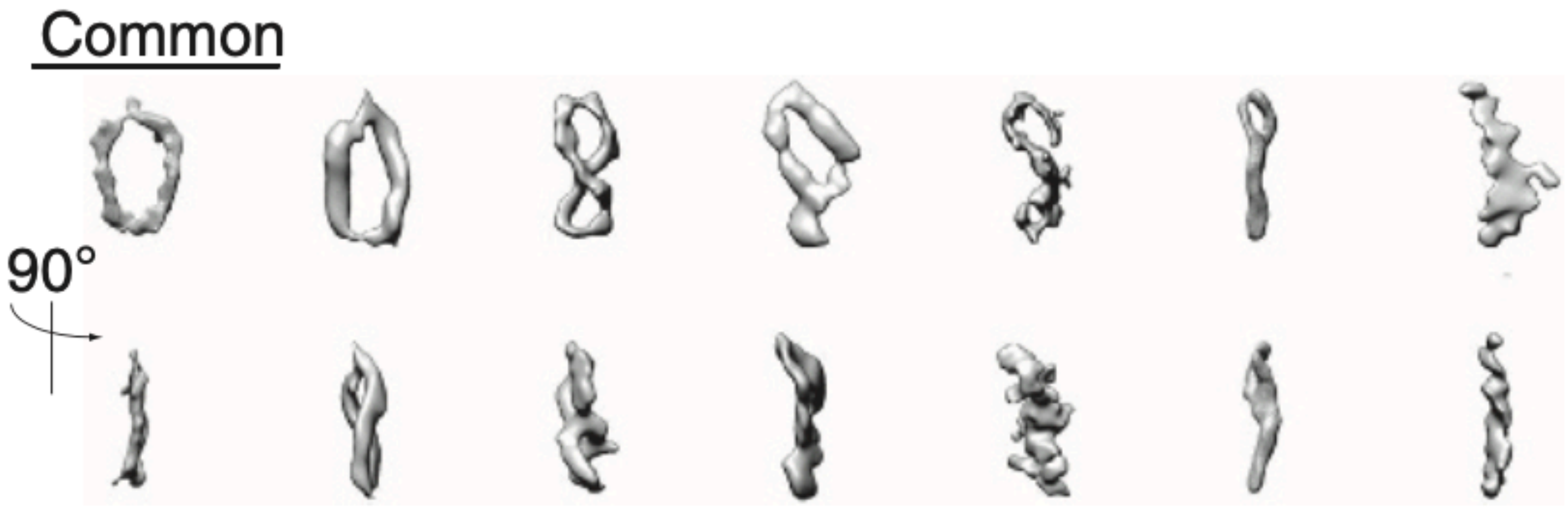


Coleman & Swigon, *J. Elasticity* (2000)

R. Waszkiewicz, M. Ranasinghe, J.M. Fogg, D.J. Catanese, M.L. Ekiel-Jeżewska, M. Lisicki, B. Demeler, E.L. Zechiedrich, P. Szymczak., *Nucl. Acids. Res.* (2023)



Cryo-EM Experiment



Cryo-EM Irobalieva et al., *Nat. Comm.* **6**, 8440 (2015)

Hydrodynamics of DNA: Diffusion & sedimentation

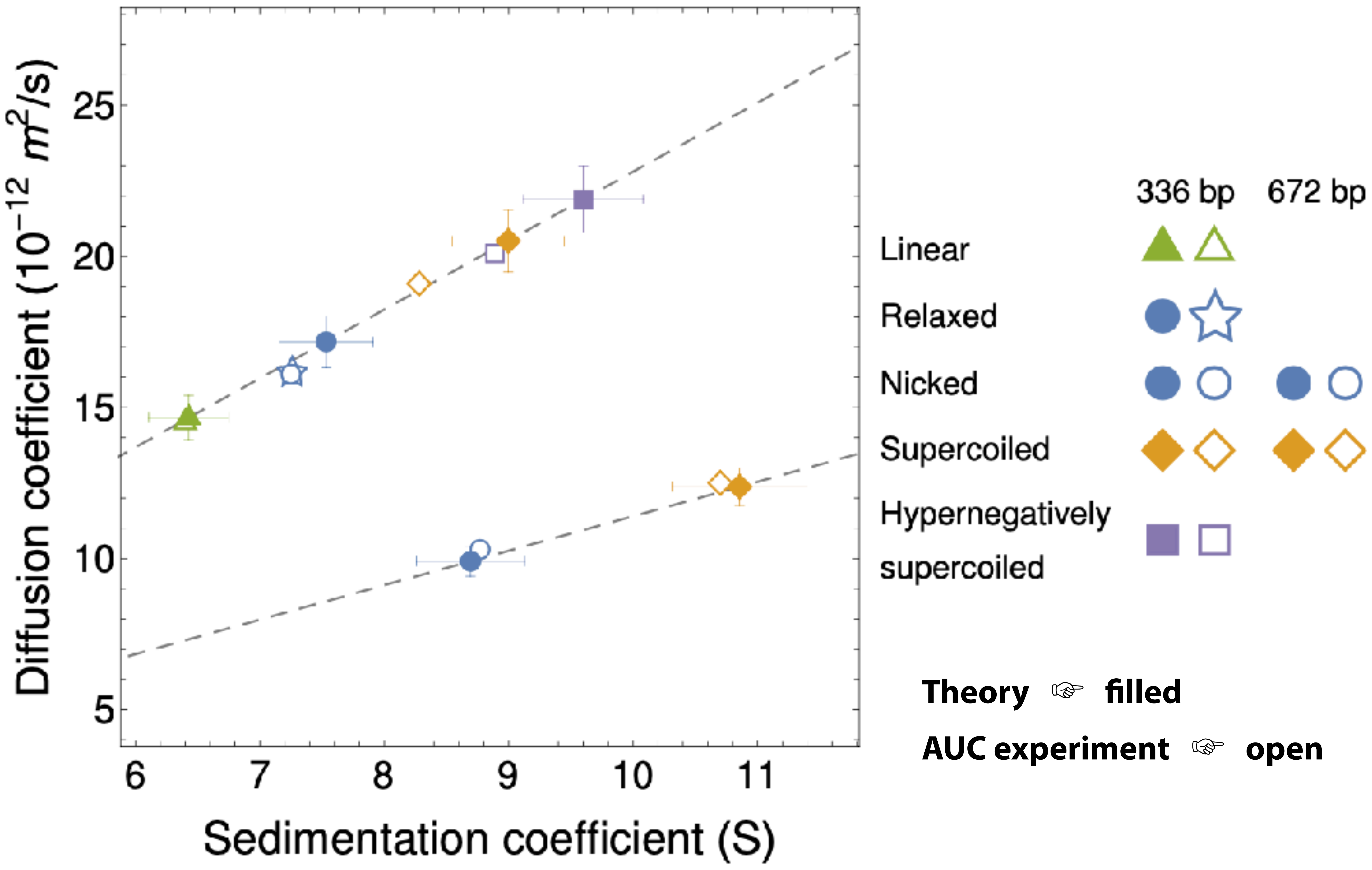
Bead-model + ZENO Stokes flow solver ☞ Hydrodynamic radius R

Diffusion ☞ Stokes-Einstein relationship

$$D = \frac{k_B T}{6\pi\eta R}.$$

Sedimentation ☞ Svedberg equation

$$\frac{s}{D} = \frac{M(1-\bar{v}\rho)}{N k_B T}.$$

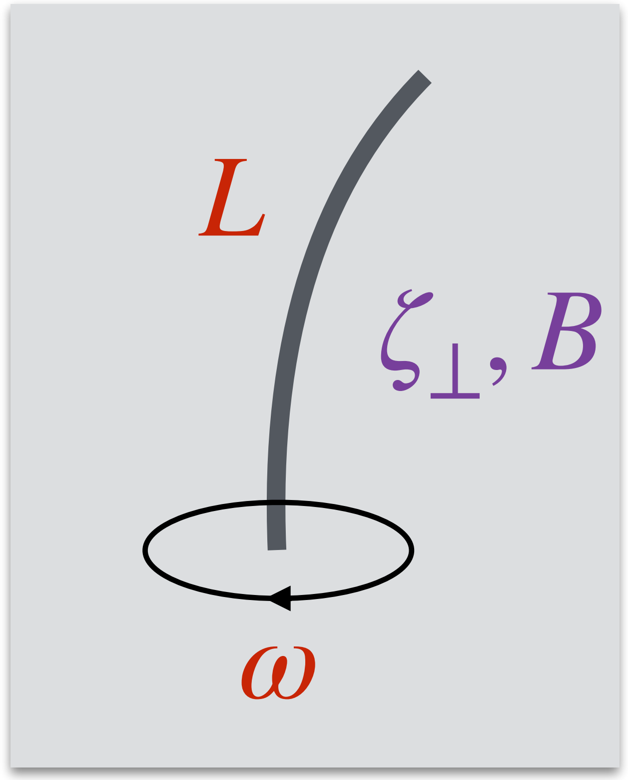


Theory ☞ filled

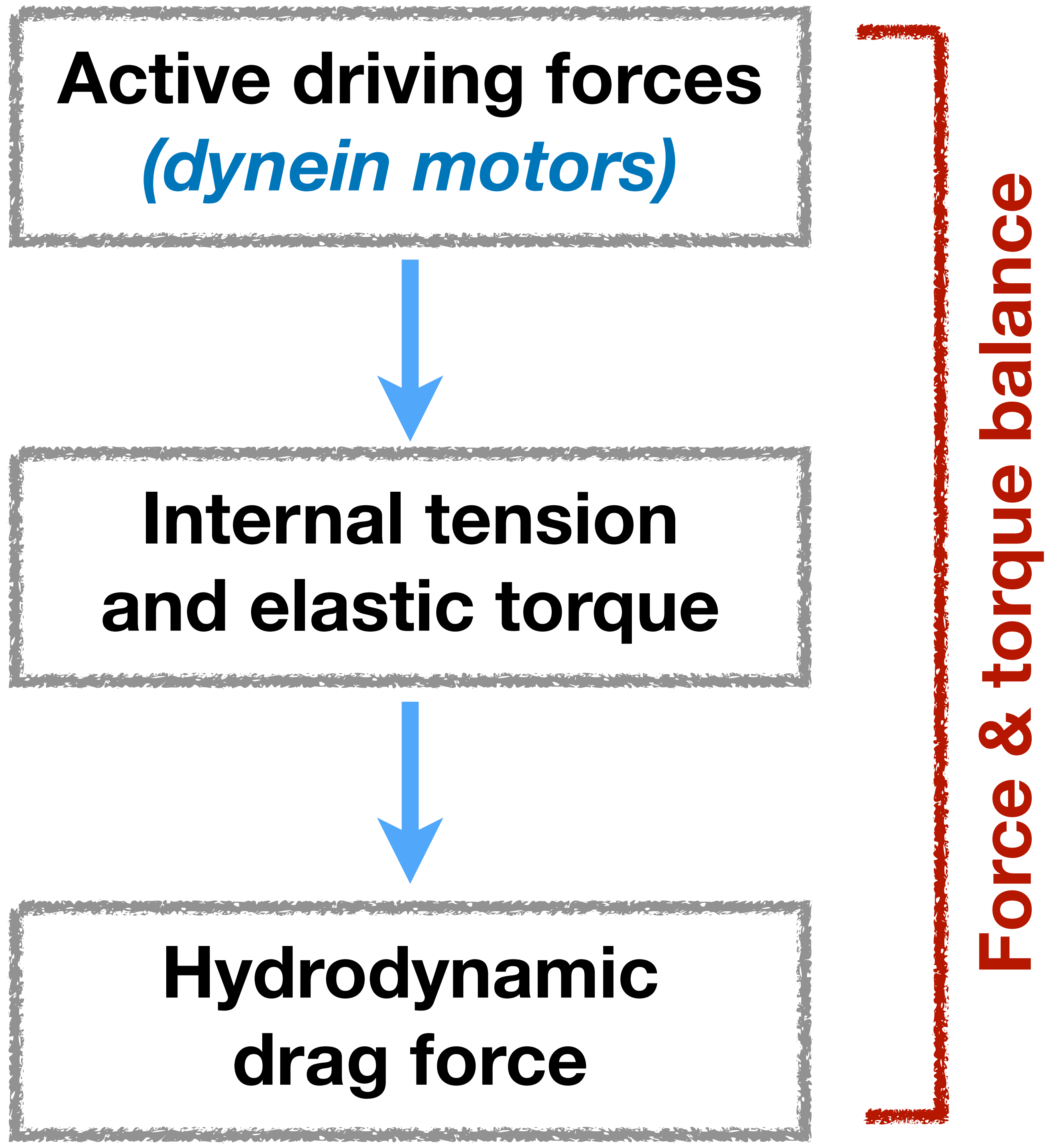
AUC experiment ☞ open

Waszkiewicz et al., Nucl. Acids Res. (2023)

Dynamics: the optimal active cilium



Force balance: Kirchhoff equations

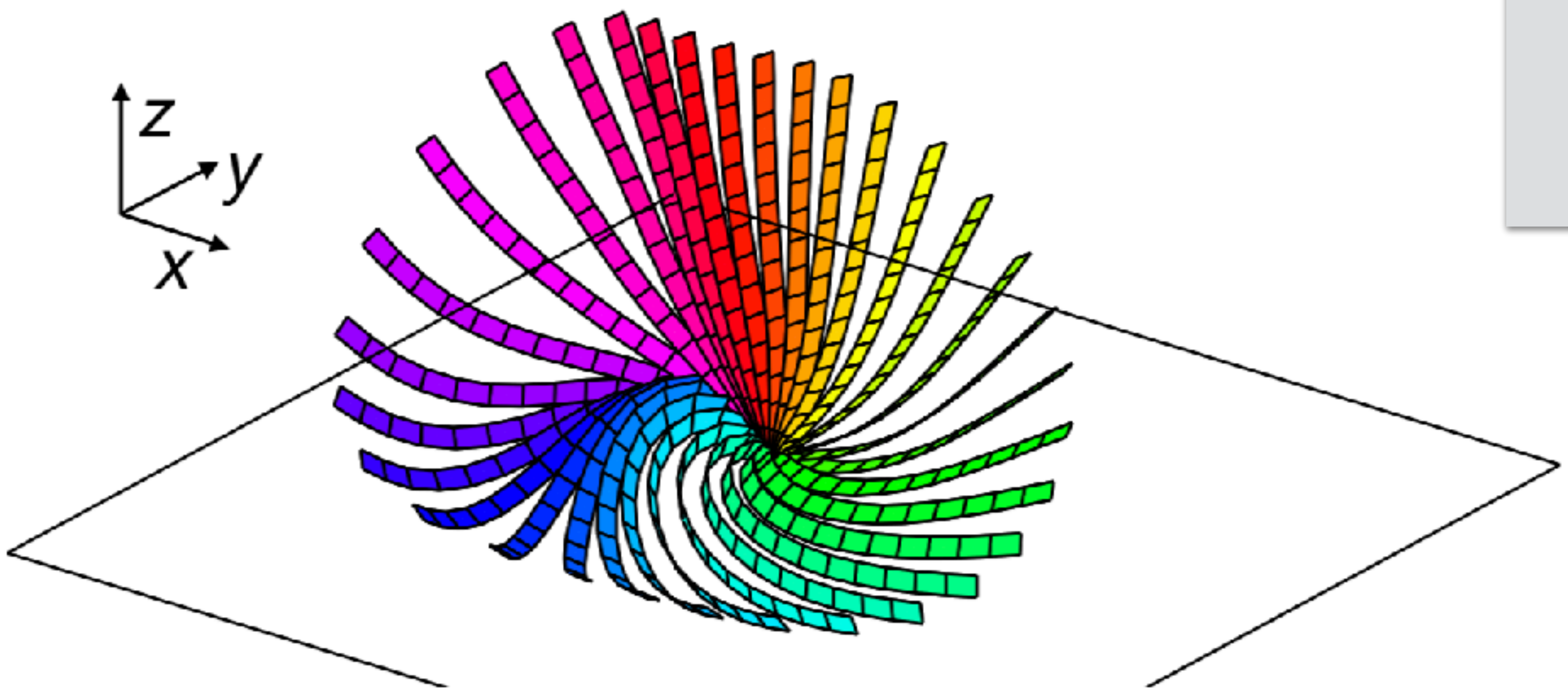


Active driving forces
(dynein motors)

Internal tension and elastic torque

Hydrodynamic drag force

Force & torque balance



Eloy & Lauga (2012)

For a given filament length and thickness, one parameter determines the motion:

$$\mathrm{Sp} = L\left(\frac{\omega\zeta_\perp}{B}\right)^{1/4}$$

Sperm number

drag vs. stiffness

$$(\omega L) \times (\zeta_\perp L)$$

$$B/L^2$$

Beating pattern crucially depends on the Sperm number of the cilium
Elastohydrodynamic optimal efficiency models resemble experimental beating patterns

An example of artificial droplet swimmers

nature physics

ARTICLES

https://doi.org/10.1038/s41567-021-01291-3

Rechargeable self-assembled droplet microswimmers driven by surface phase transitions

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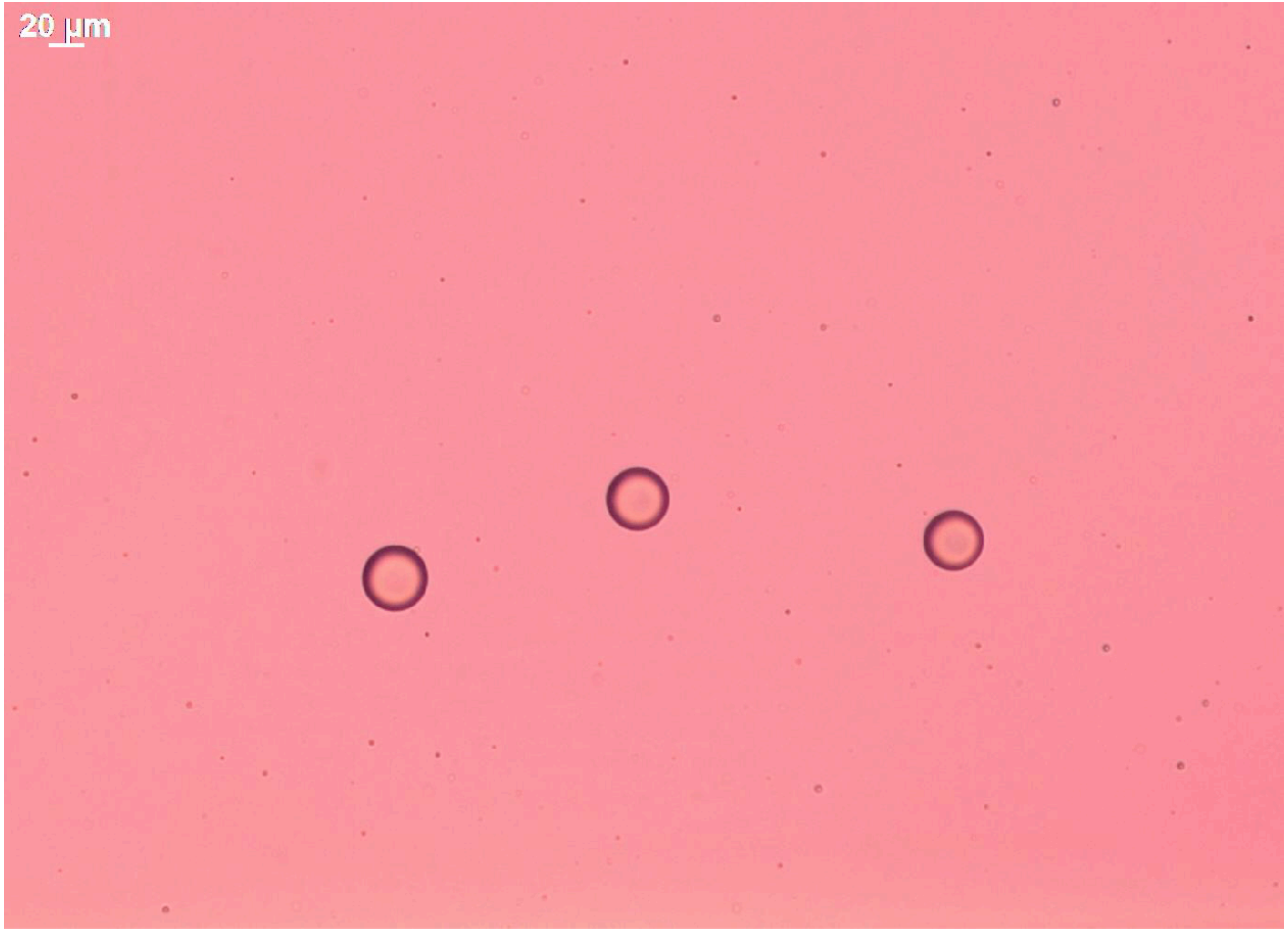
Simple mixture:

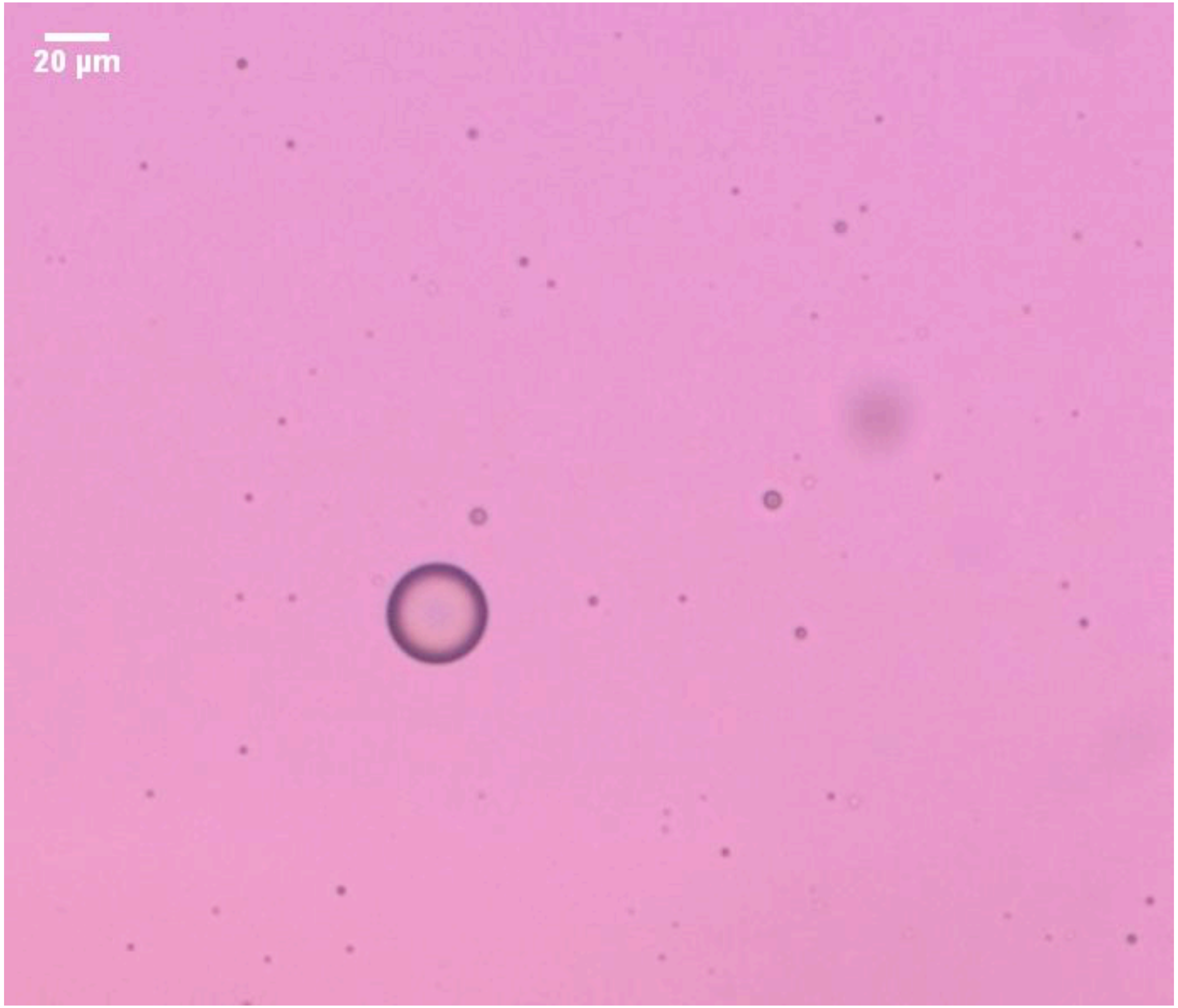
1) **Water**
2) **Alkane oil drops** [tetradecane or pentadecane]
3) **Surfactant** [~1.5wt% aqueous surfactant solution (Brij 58)]

+ ca. 5 K temp. oscillations

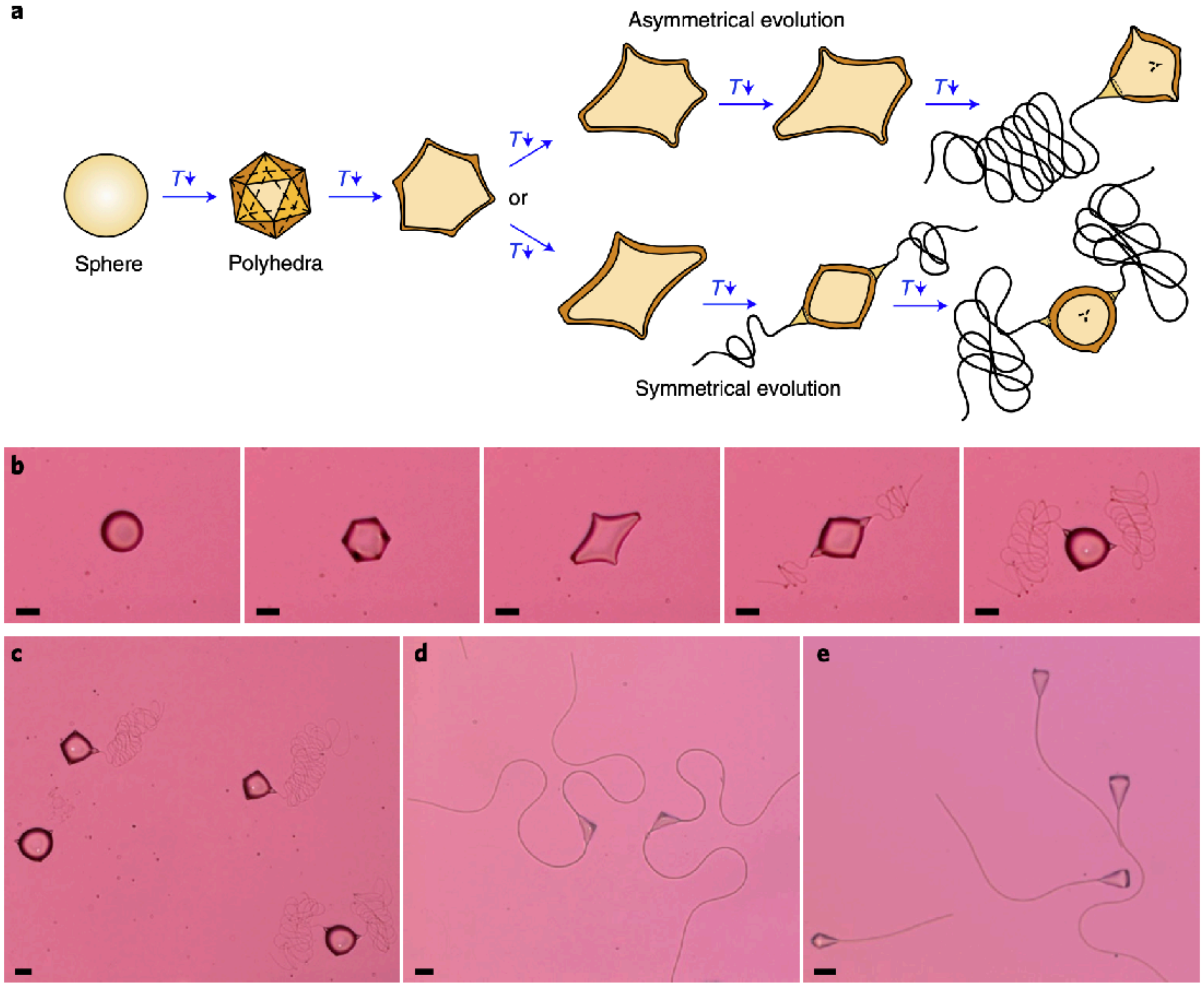
Droplet swimmers



Droplet swimmers



Formation of asymmetric droplets



Hydroelasticity of extruded filaments

Elastic energy of the filament

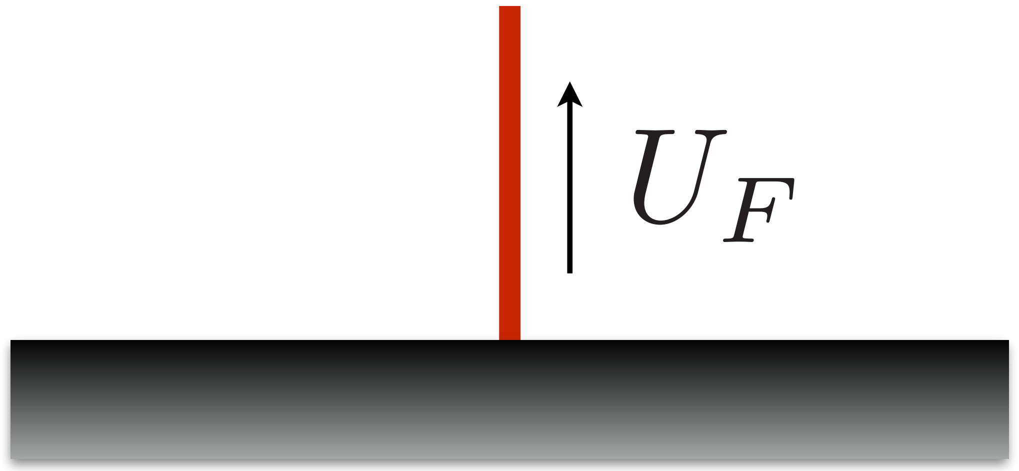
$$\mathcal{E} = \frac{1}{2}\int_0^L [A(\boldsymbol{r}_{ss}\cdot\boldsymbol{r}_{ss}) + \sigma(\boldsymbol{r}_s\cdot\boldsymbol{r}_s)]\mathrm{d}s,$$

Buckling length

$$\ell = \left(\frac{A}{\zeta_{\parallel}U_F}\right)^{1/3}$$

Elastic force density $\boldsymbol{f}_e = -A\boldsymbol{r}_{ssss} + (\sigma\boldsymbol{r}_s)_s$

Drag force density $\boldsymbol{f}_h = -[\zeta_{\parallel}\boldsymbol{tt} + \zeta_{\perp}\boldsymbol{nn}]\cdot\boldsymbol{r}_t$



Filament extrusion $$\frac{D\boldsymbol{r}}{Dt} = U_F\boldsymbol{t} + \frac{\partial\boldsymbol{r}}{\partial t}$$

Force balance condition (Stokes flow) $\boldsymbol{f}_e + \boldsymbol{f}_h = \boldsymbol{0}$

Final set of equations $\sigma(s) \quad \& \quad \theta(s)$

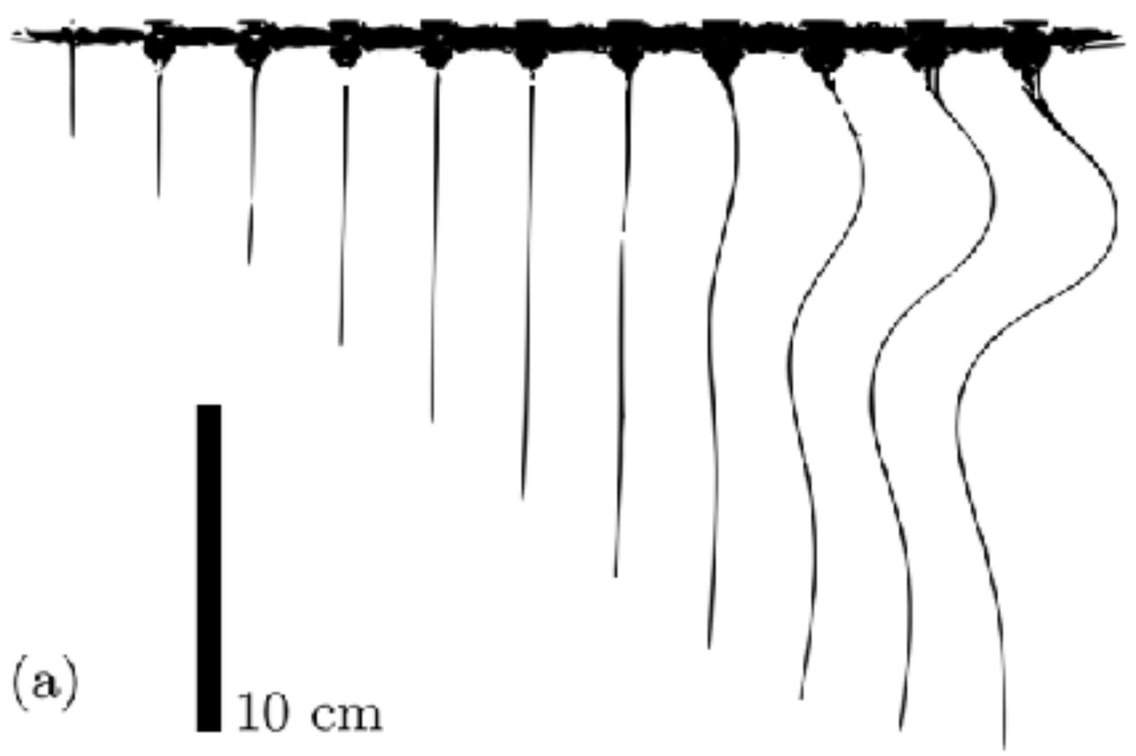
$$\eta\theta_t = -\theta_{ssss} + [3(1+\eta)\theta_s^2 + \sigma]\theta_{ss} + (1+\eta)\sigma_s\theta_s - \eta\theta_s,$$

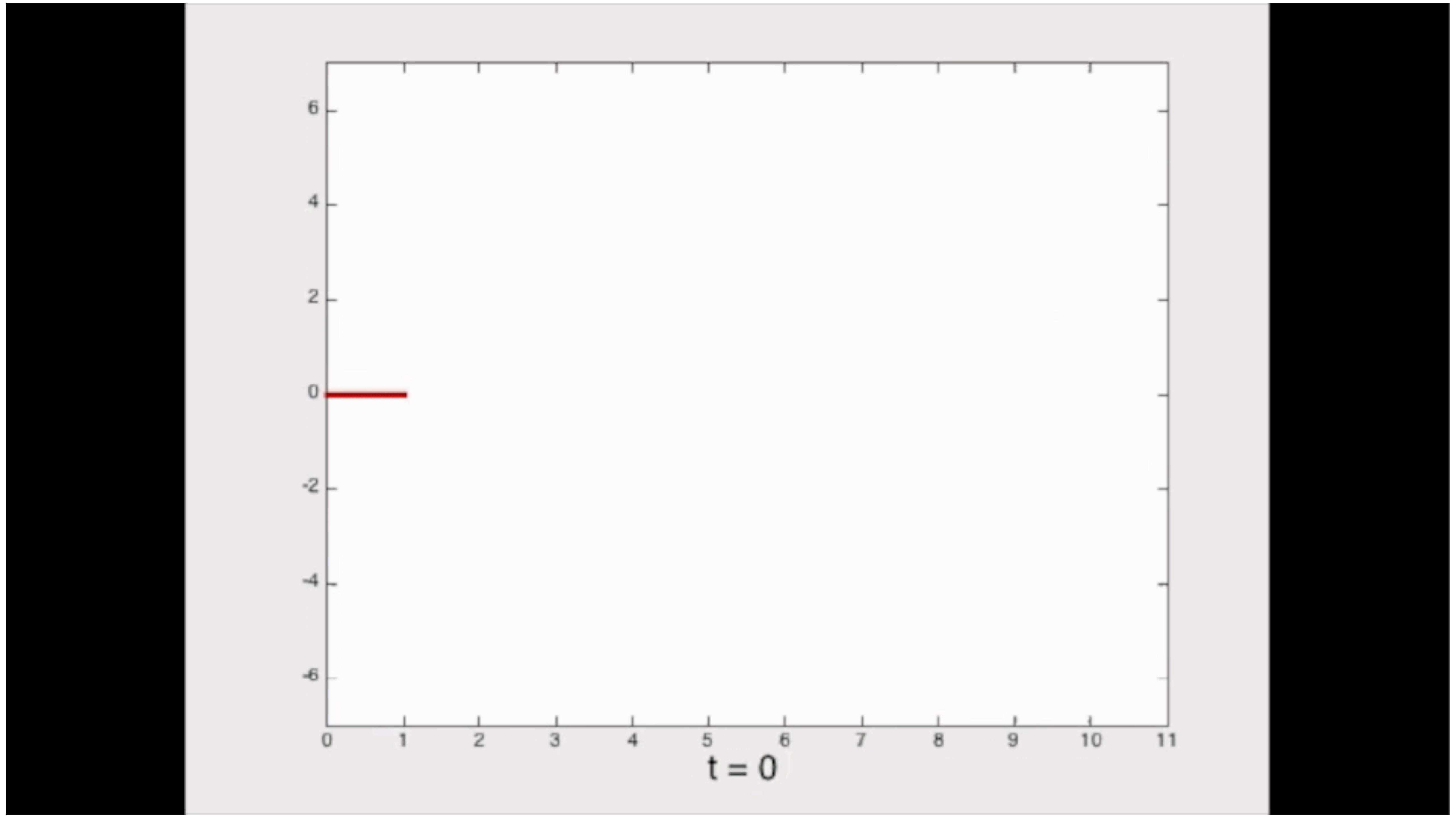
$$\eta\sigma_{ss} - \theta_s^2\sigma = \theta_s^4 - (3\eta+1)\theta_s\theta_{sss} - 3\eta\theta_{ss}^2.$$

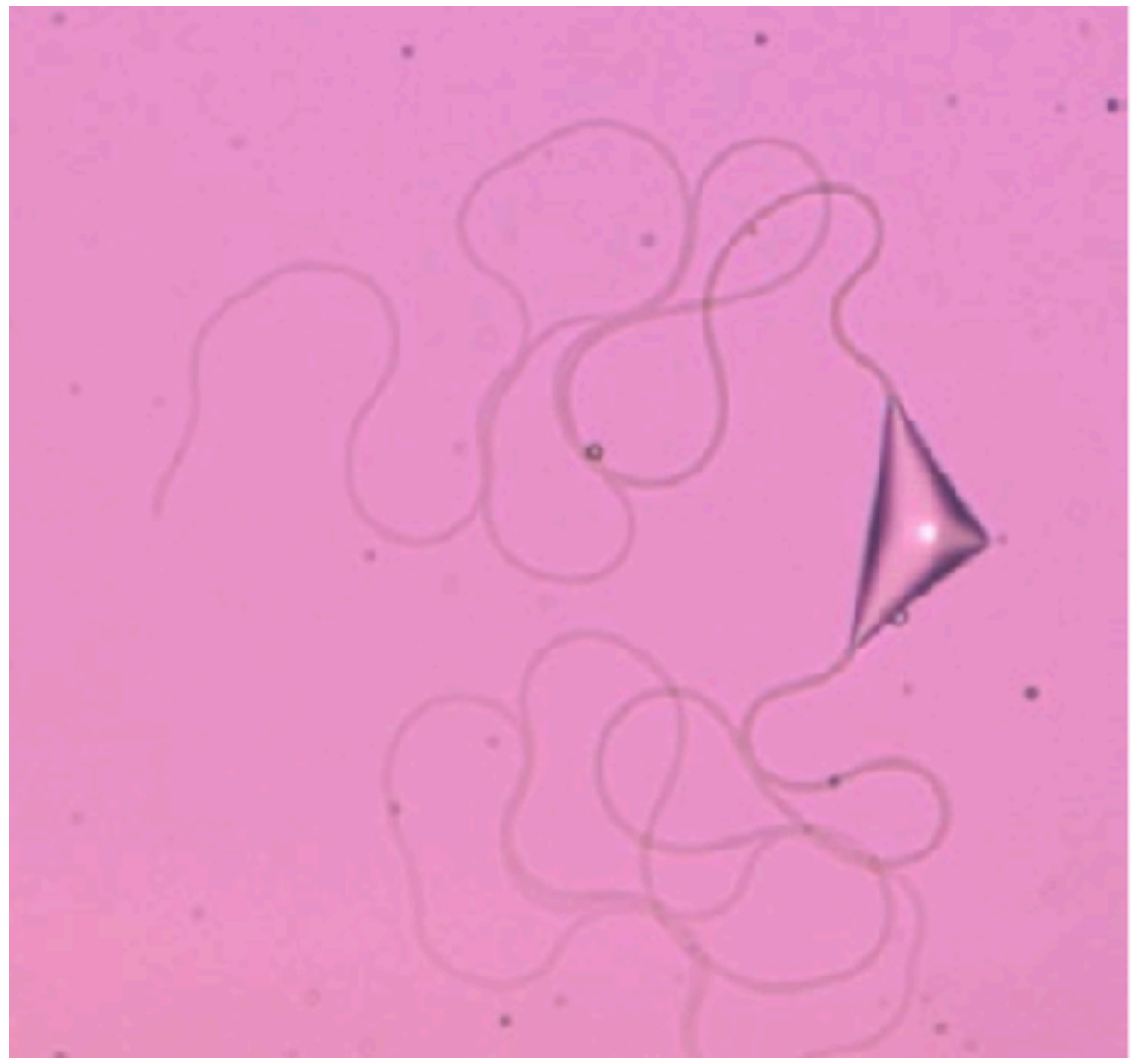
Buckling dynamics of extruded filaments

Extrusion of an elastic string into a viscous fluid: competition between drag and deformation

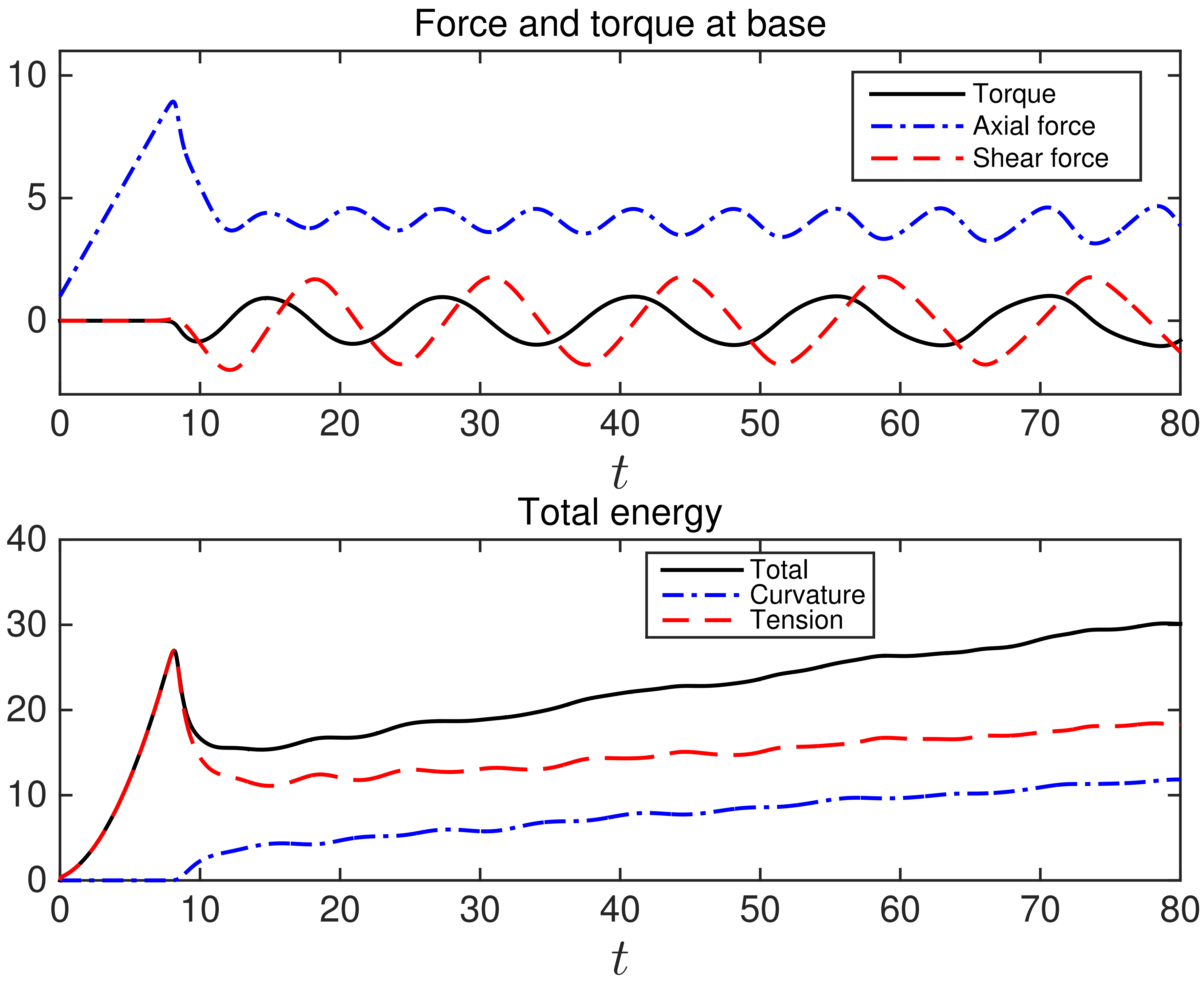
Experiment: *Gosselin et al. (2014)*







Buckling dynamics of extruded filaments



- **Initial extrusion limited by buckling**
- **Long-time stable oscillations**

Simple model of a swimmer

Scaling analysis

Tension at short times (before buckling)

$$\sigma \sim \zeta_{\|} L(t) U_F \sim \zeta_{\|} U_F^2 t$$

Tension after buckling:

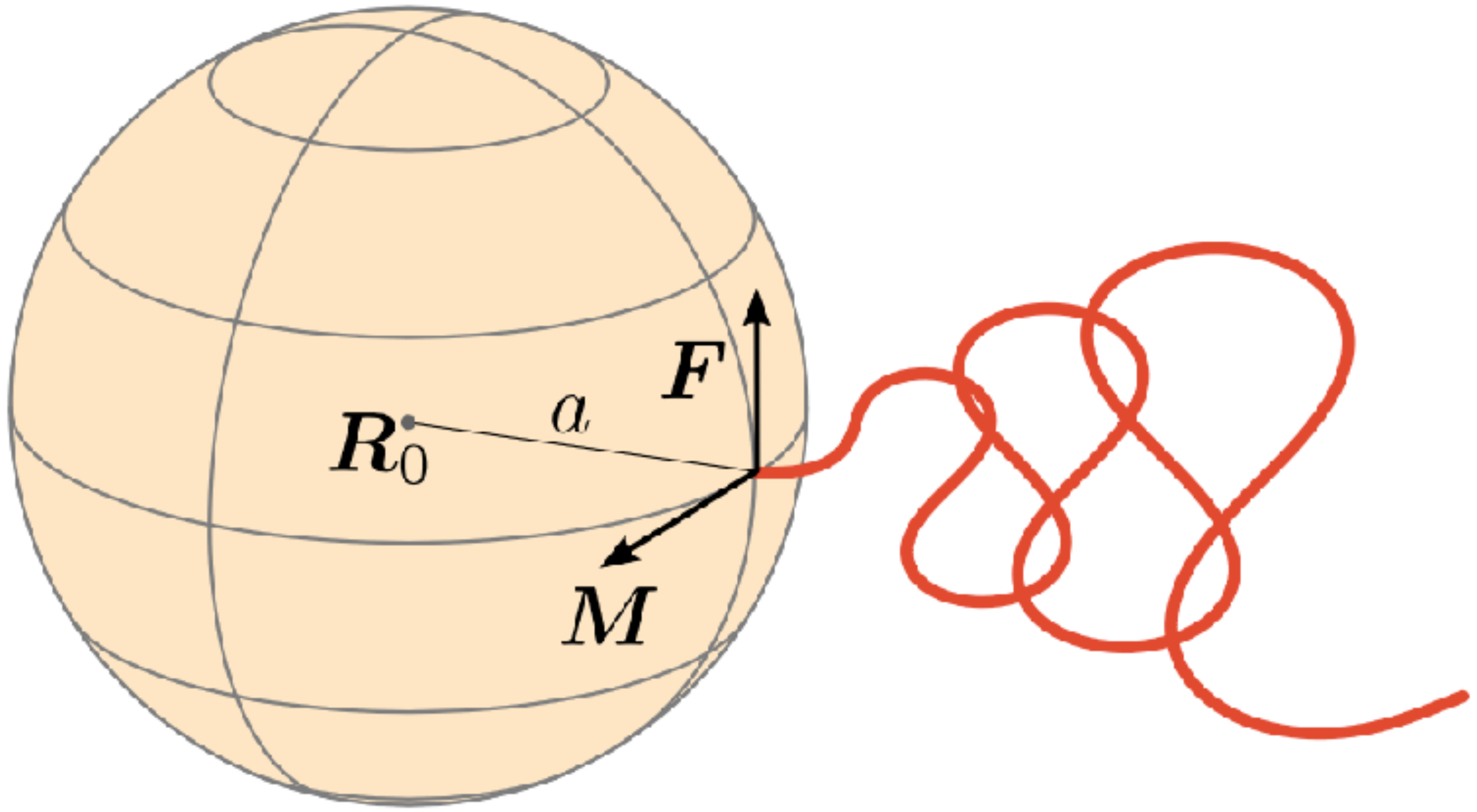
$$\sigma \sim A\ell^{-2} \sim (A\zeta_{\|}^2 U_F^2)^{1/3}$$

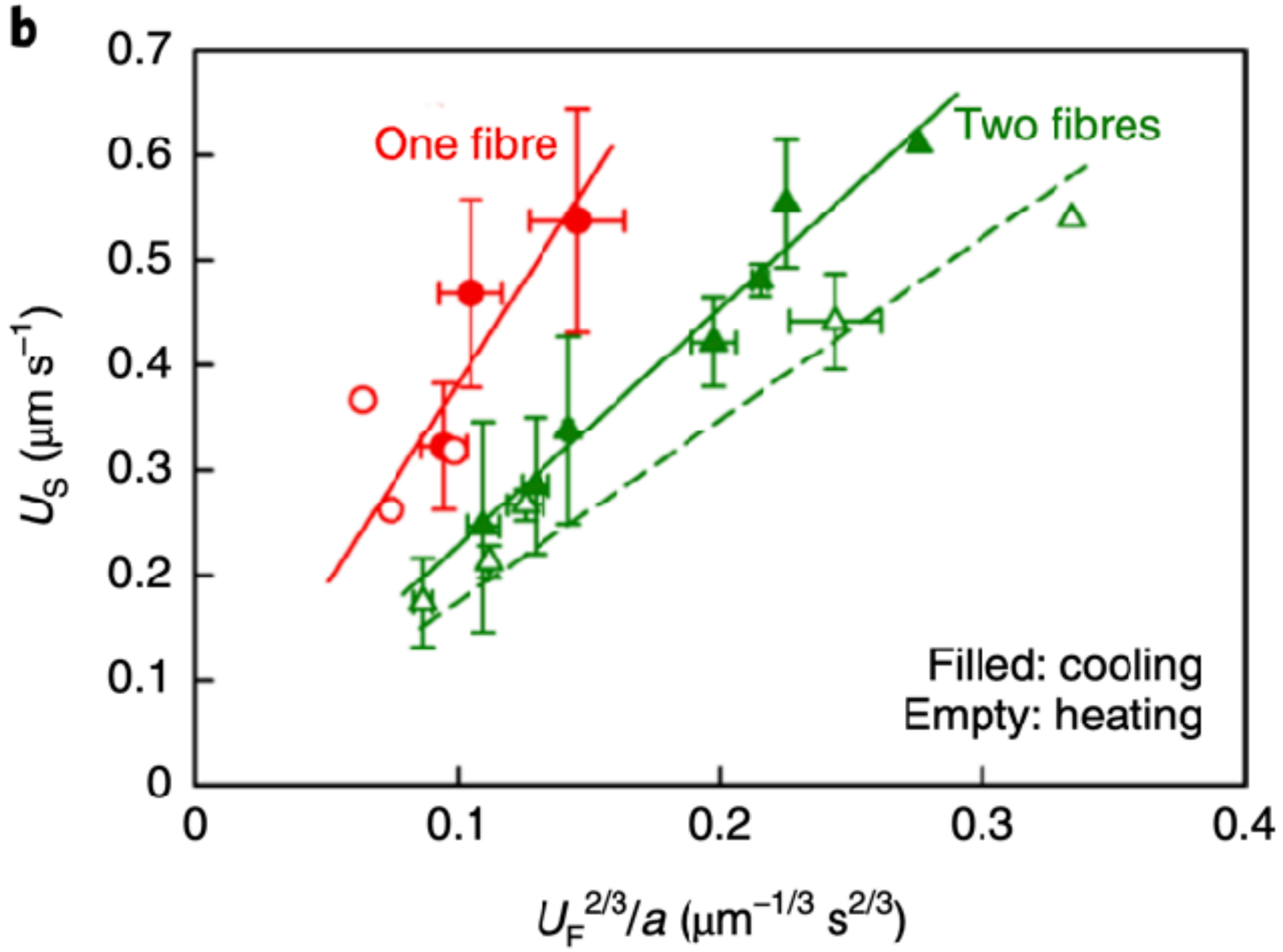
Tension balancing drag = swimming

$$\sigma \sim \mu a U_S$$

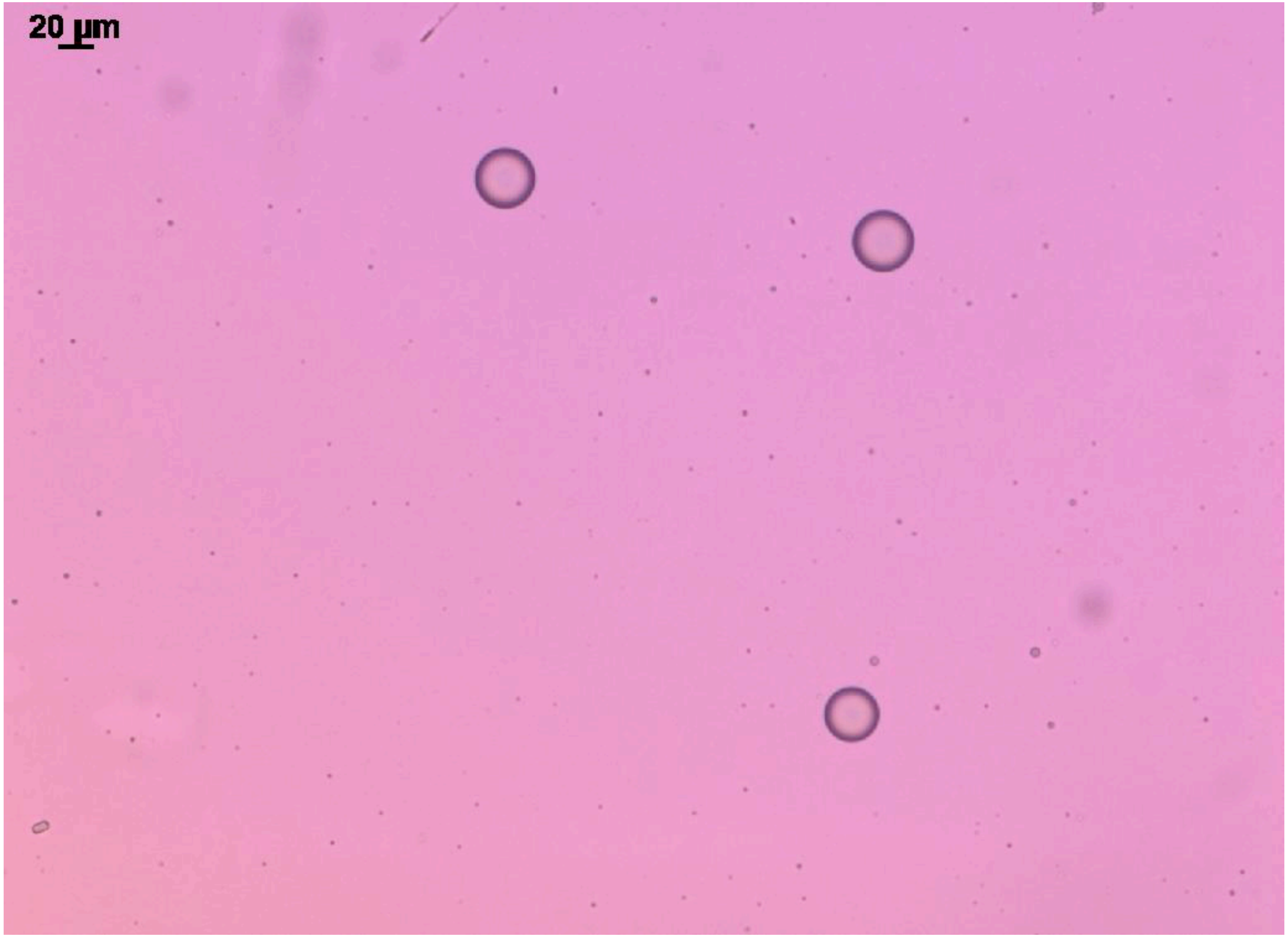
Swimming scaling relationship

$$\boxed{\frac{U_S}{U_F} \sim \frac{(A\zeta_{\|}^2 U_F^2)^{1/3}}{\mu a U_F} = \frac{\ell}{a}}$$

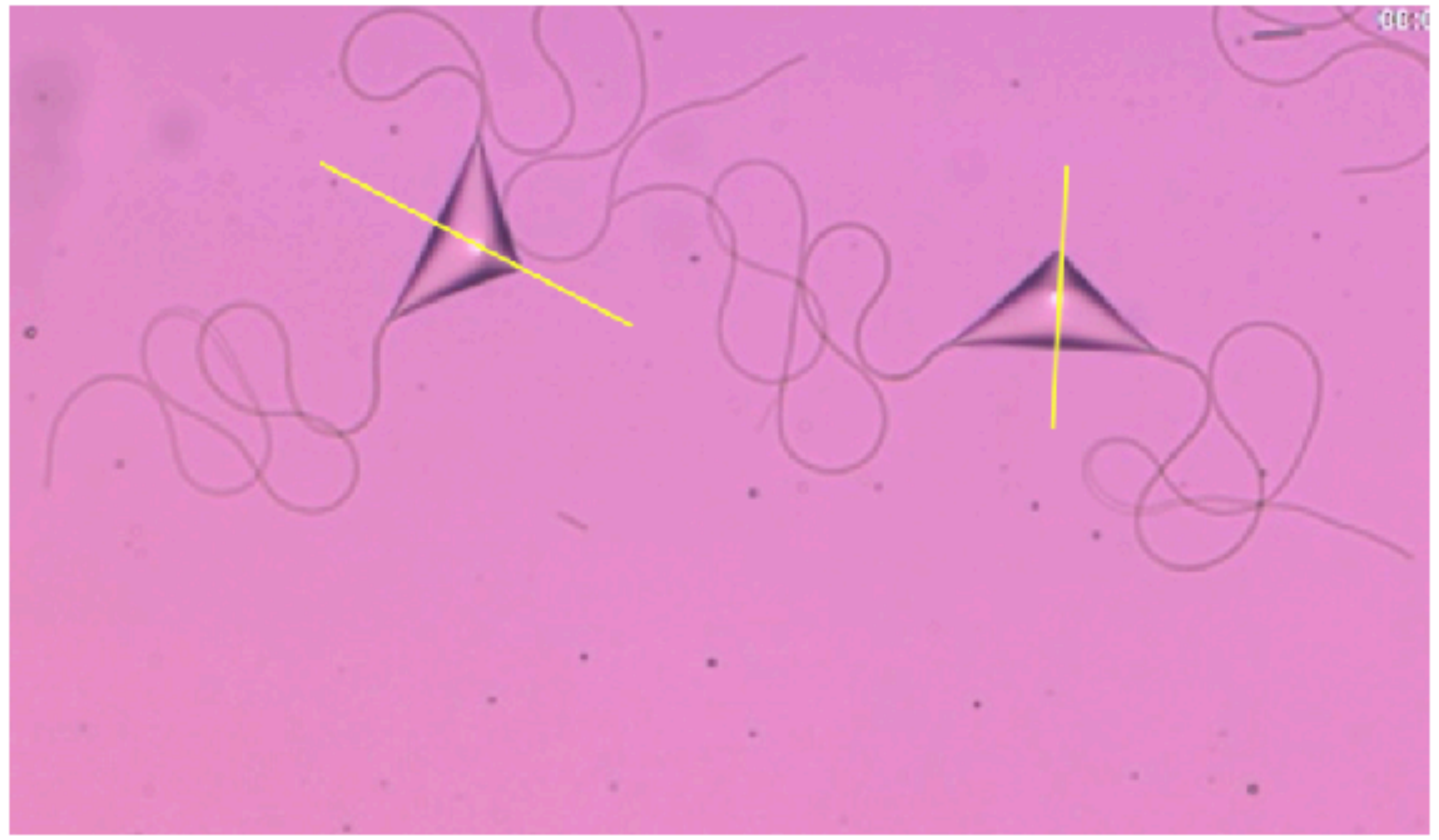


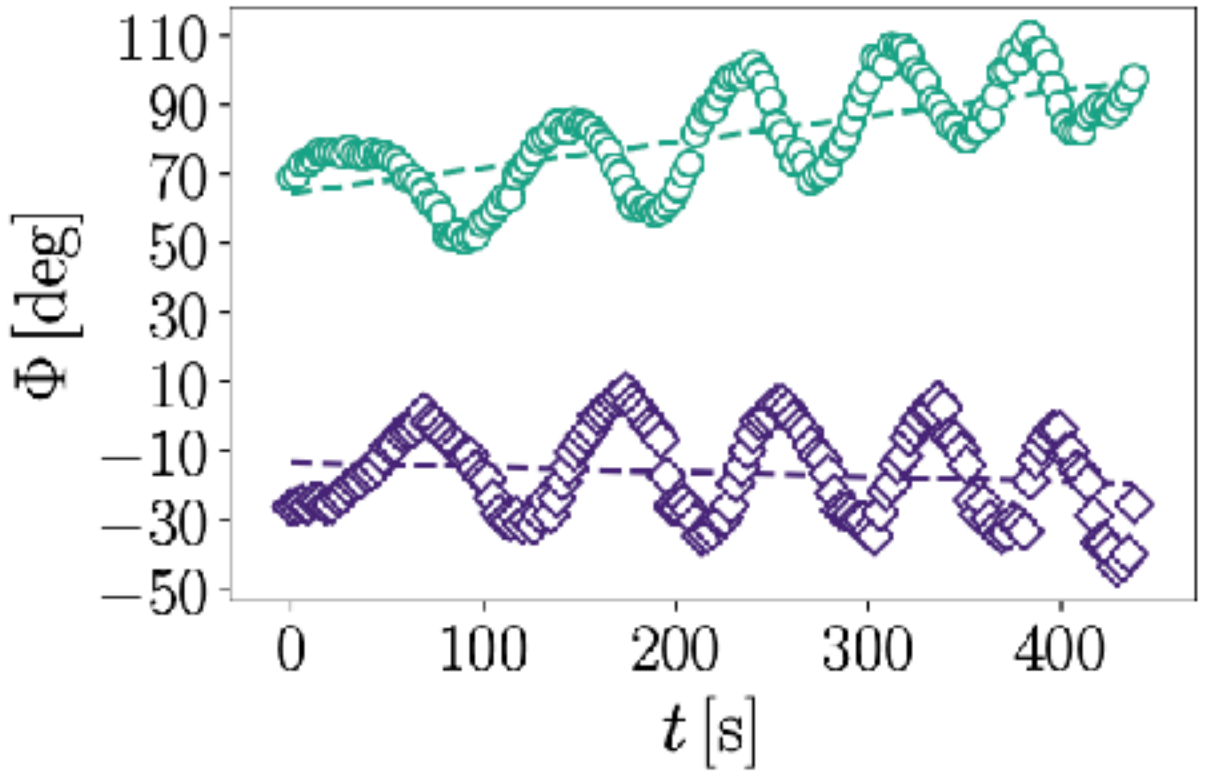


Tracking the droplets

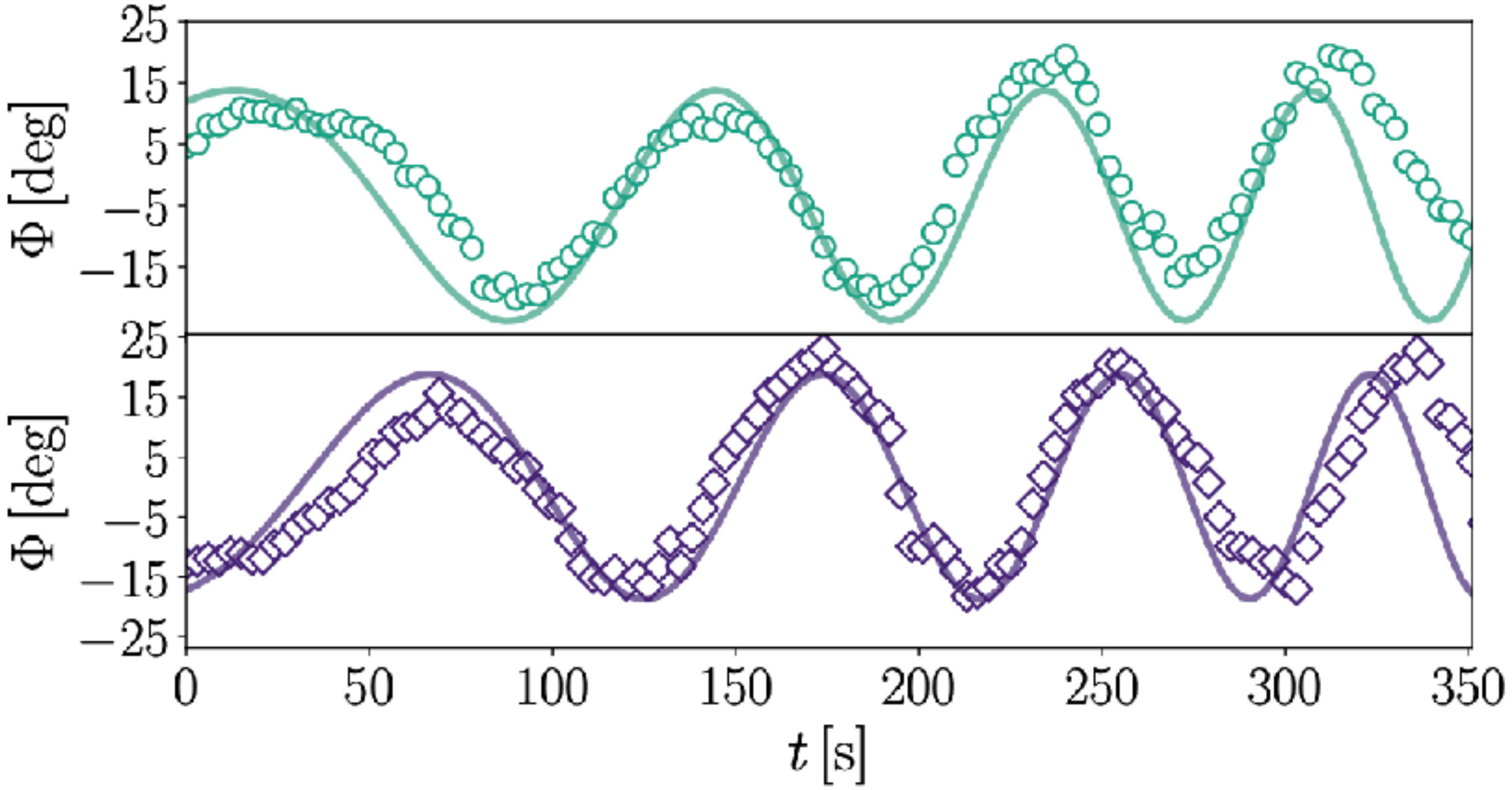


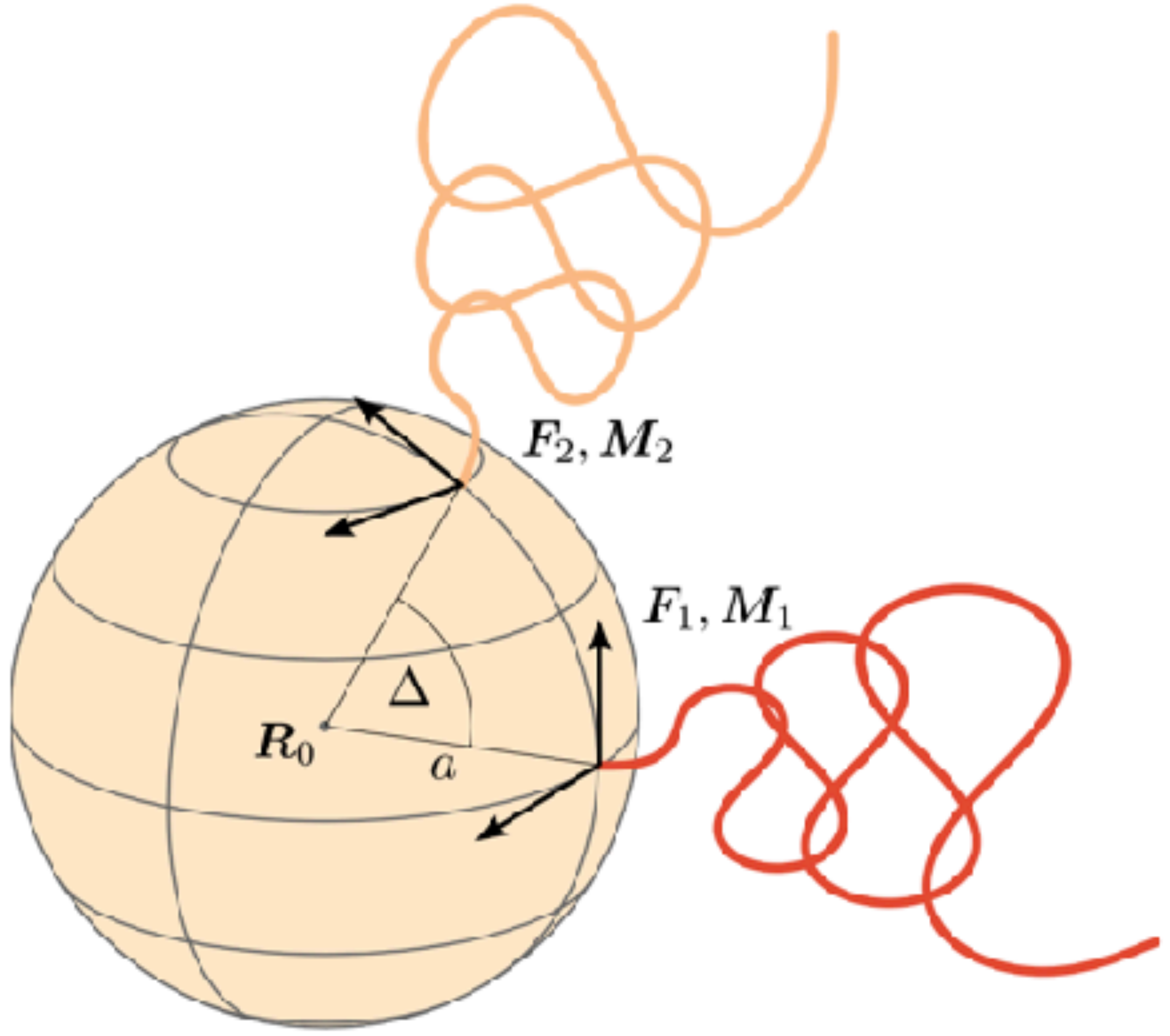
Two-tailed swimmers





no phase shift;
no hydrodynamic
synchronisation

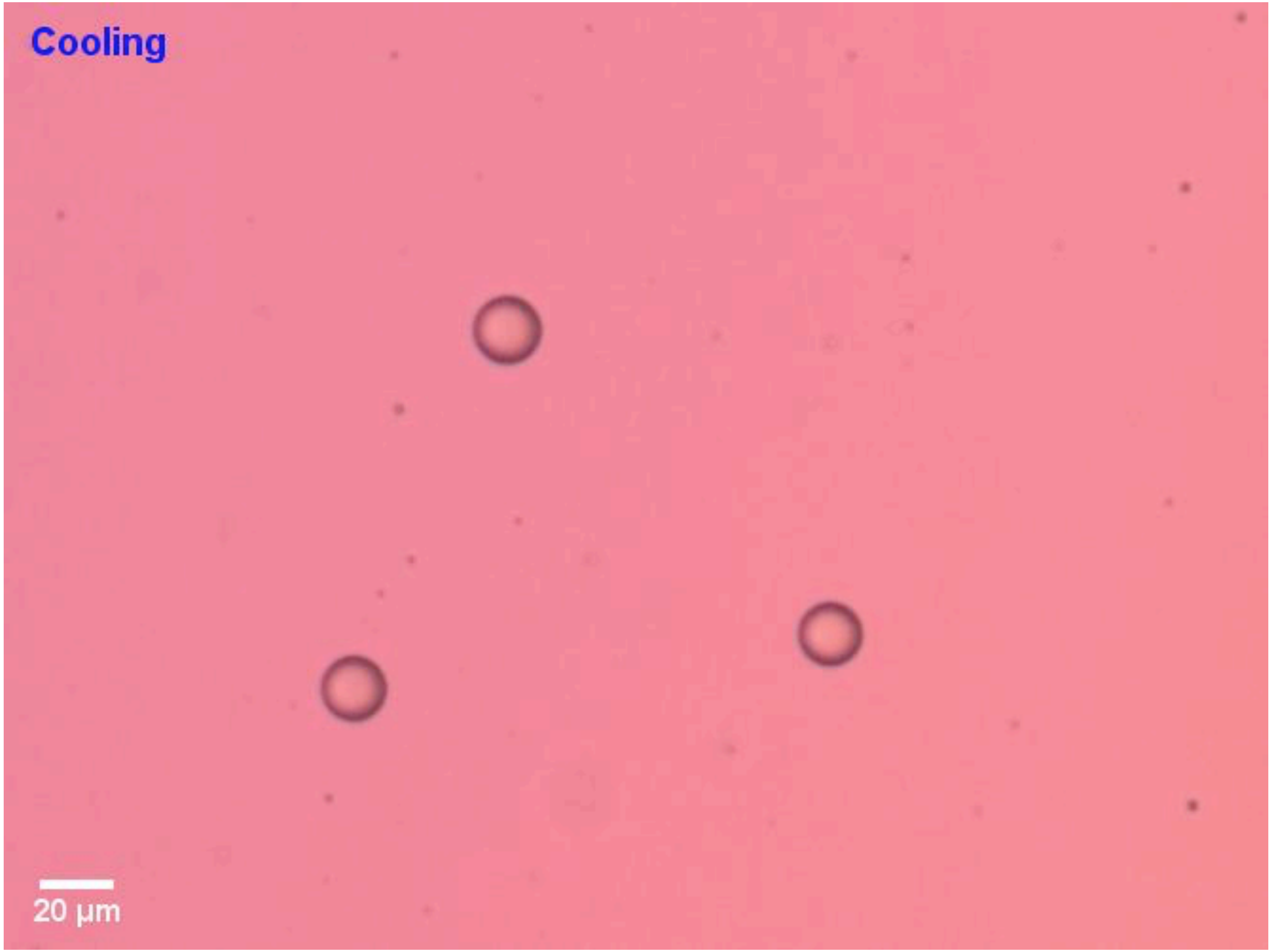




Two-tail model joins contributions (force and torque) from two independent tails

Semi-empirical theory predicts the correct behaviour of droplet swimmers

Reversible filament extrusion (recharging)



Conclusions

- Microscale swimming results from balance between propulsion forces and viscous fluid drag at low Reynolds number
- **Universal properties of Stokes flows** pose limitations on propulsion mechanisms
- Elasticity of macromolecules affects their hydrodynamic properties. The shape of **supercoiled DNA** can be inferred from elastic beam models. Elastic models grasps shape stability & aids sedimentation/diffusion predictions
- Exemplary artificial swimmers – **rechargeable droplet microswimmers driven by internal phase transitions** – simple and inexpensive
- Droplet dynamics governed by extruding elastic filaments and their buckling dynamics. Elastohydrodynamic model quantitatively captures swimming speed

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