Propulsion with stiff polymers

Manoel Manghi (Toulouse)	PRL 96, 068101 (2006)
Yong-Woon Kim (UCSB)	PRL in press (2006)
X. Schlagberger, Roland Netz (TUM)	

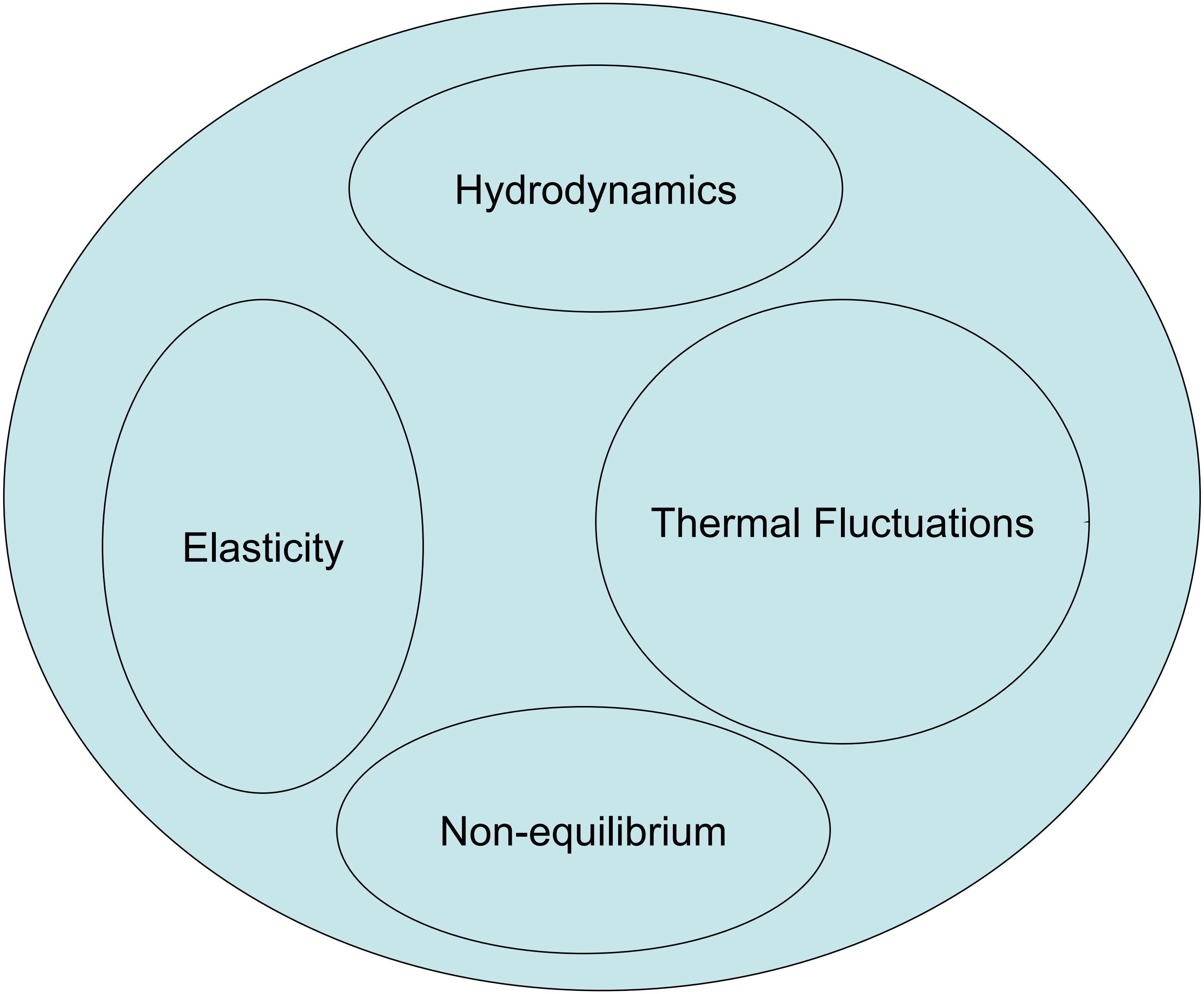
1) sedimentation of polymers

2) electrophoresis of polymers

3) polymers in shear flow (unfolding of proteins in blood flow)

4) polymers at surfaces in shear or electric fields
   (glycocalix deformation under shear)

5) driven stiff polymers -> propulsion



Hydrodynamics

Elasticity

Thermal Fluctuations

Non-equilibrium

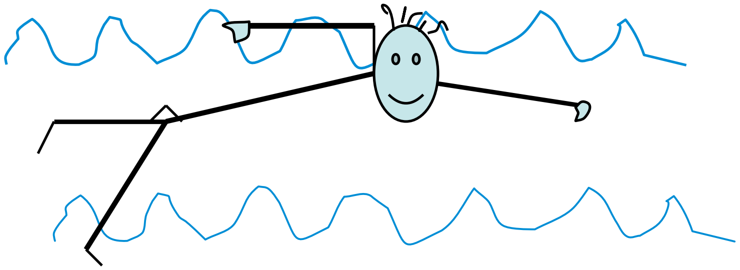
Hydrodynamics at low Reynolds numbers

Stationary Navier-Stokes equation $\eta\,\Delta\vec{v}(\vec{r}) - \nabla p = \cancel{\rho(\vec{v}\cdot\nabla)\vec{v}}$

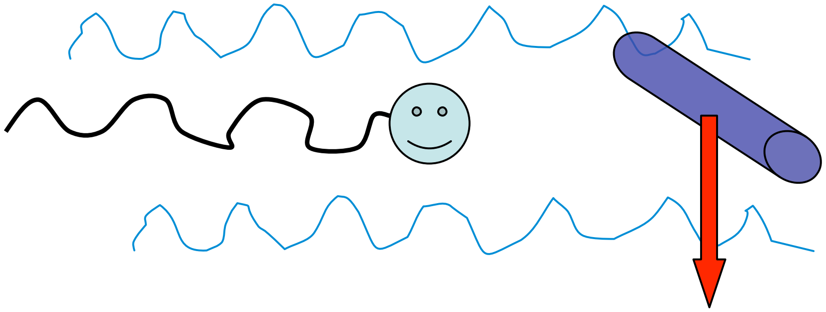
If the Reynolds number $Re^{tr} = \frac{\rho}{\eta}\, l\, v \ll 1$, $Re^{rot} = \frac{\rho}{\eta}\, r^2\, \omega \ll 1$,

one obtains the **creeping flow equation.**

<u>human</u>



<u>bacterium</u> <u>sinking cylinder</u>

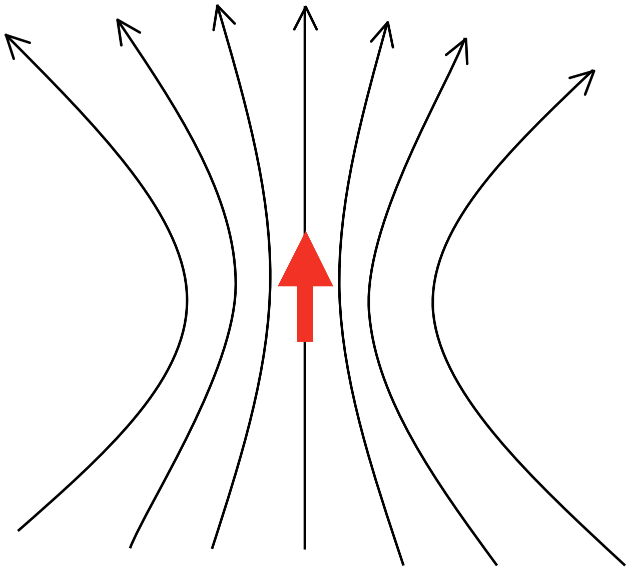


H_2O: $\eta = 0.001$ Pa s;
$\rho = 1000$ kg/m^3
v = 1 m/s
l = 1 m

$\Big\}$ Re = 10^6

v = 10^{-5} m/s
l = 1 μ
→ Re = 10^{-5}

v ~ 10^{-7} m/s
l = 1 μ
→ Re = 10^{-7}



flow-field due to point-force at origin:

$$u^{\alpha}(r) = H^{\alpha\beta}(r)\, f^{\beta}$$

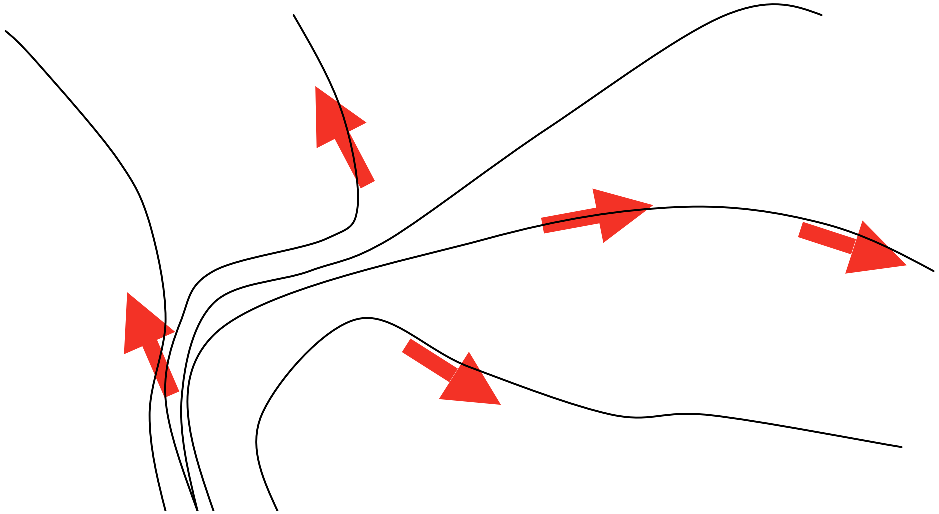
α,β =1,2,3

$$H^{\alpha\beta}(r) = \frac{1}{8\pi\eta r}\left[\delta_{\alpha\beta} + \hat{r}^{\alpha}\,\hat{r}^{\beta}\right]$$

(Oseen-Tensor)

for many particles the superposition principle is valid:

$$u^{\alpha}(r) = \sum_{i} H^{\alpha\beta}(r - r_i)\, f_i^{\beta}$$



invert to get forces for prescribed solvent velocity distribution !!

Next: add thermal noise

Theoretical Framework: Position Langevin Equation

Velocity of i-th particle:

$$\boxed{\cancel{m\ddot{r}_j(t)\overleftrightarrow{\mu}_{ij}} + \dot{r}_i(t) = \overleftrightarrow{\mu}_{ij}\; f_j(t) + \xi_i(t)}$$

deterministic force

$$f_j(t) = -\partial U(t)/\partial r_j(t) + E$$

Random force

$$\left\langle \xi_i(t)\,\xi_j(t')\right\rangle = 6\,\overleftrightarrow{\mu}_{ij}\;k_B T\;\delta(t-t')$$

Mobility matrix:

$$\overleftrightarrow{\mu}_{ij} = D_{ij}/k_B T = \mu_0\,\delta_{ij} + \overleftrightarrow{H}(r_i,r_j)$$

self mobility: $\mu_0 = (6\pi R\eta)^{-1}$

hydrodyn. interact.

equivalent to Smoluchowski equation for particle distribut. $W(r_j,t)$:

$$\frac{\partial W}{\partial t} = \sum_{i,j}\frac{\partial}{\partial r_i}\left[D_{ij}\frac{\partial W}{\partial r_j} - \mu_{ij} f_j W\right]$$

with solution: $W \cong e^{-U/k_B T}$

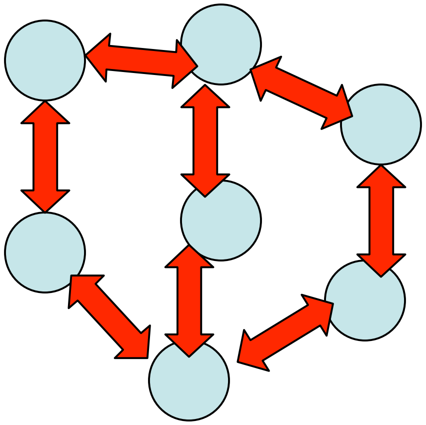
straightforward way to satisfy no-slip in multi-particle system

$$u_j^\alpha(r_j) = \sum_i H^{\alpha\beta}(r_j - r_i)\; f_i^\beta = \mu_0 f_j^\alpha + v_\infty(r_j) = v(r_j)$$

velocity of j-th
particle

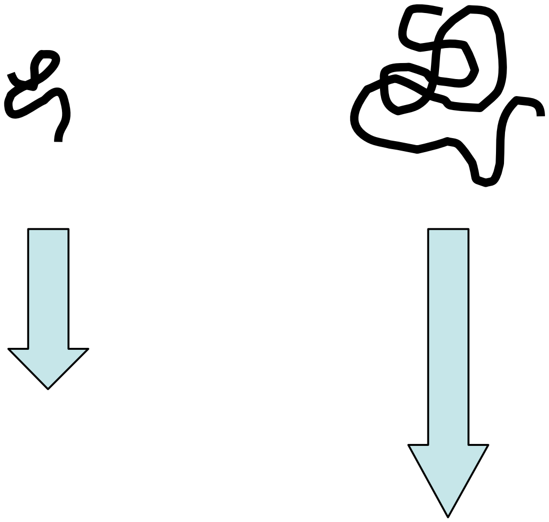
solvent-velocity
due to other particles

solvent-velocity
at particle position



cohesive/elastic forces in objects automatically lead to solvent flow stagnation a few examples ….

Separation by sedimentation in the ultracentrifuge



G: force per monomer
N: monomer number

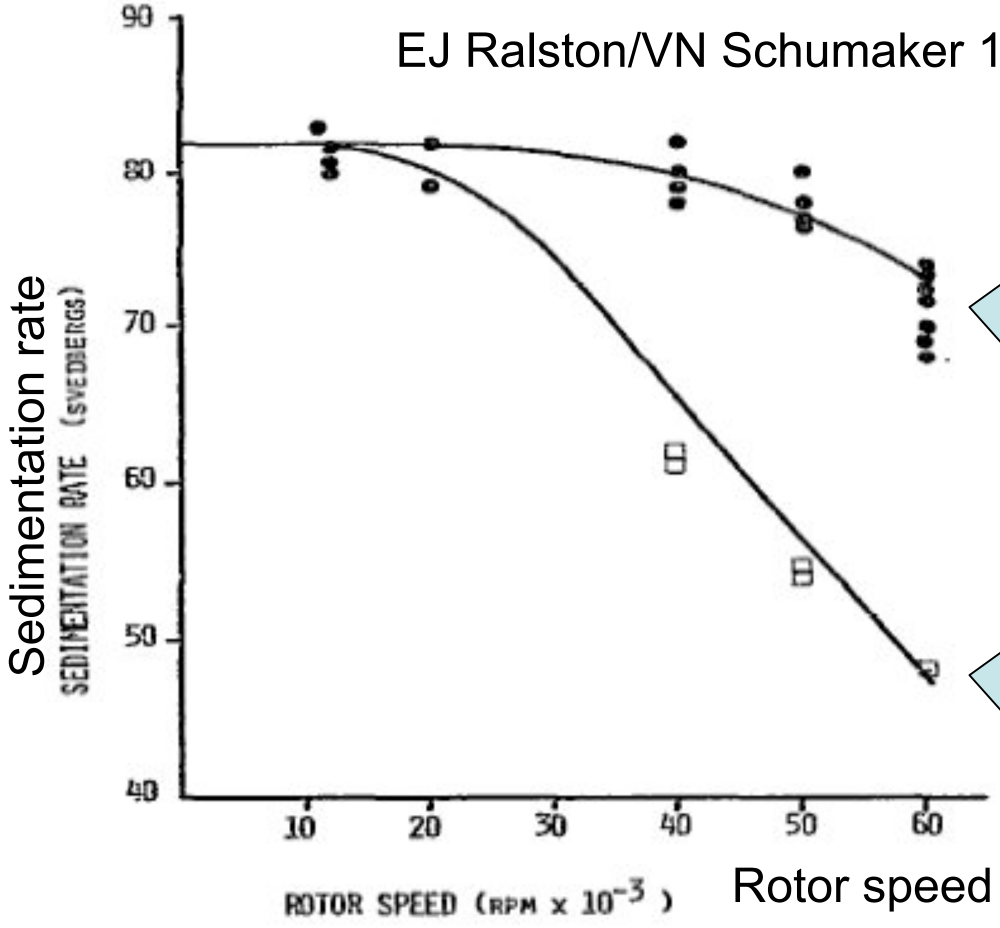
velocity $v=GN\mu$

mobility $\mu=1/6\pi\eta R=1/6\pi\eta N^{\nu}$

--> velocity $v \approx G\, N^{1-\nu}$

Why gel-electrophoresis is used for separating DNA (and not the ultracentrifuge)

- sedimentation rate of polymers goes down at high rotor speeds
- crossover is polymer-length dependent!



EJ Ralston/VN Schumaker 1979

circular episome 1338 DNA

linear episome 1338 DNA at low concentrations

Crumpling of Flexible Chains (Xaver Schlagberger)

hydrodynamic simulations of sedimenting polymers

Xaver Schlagberger

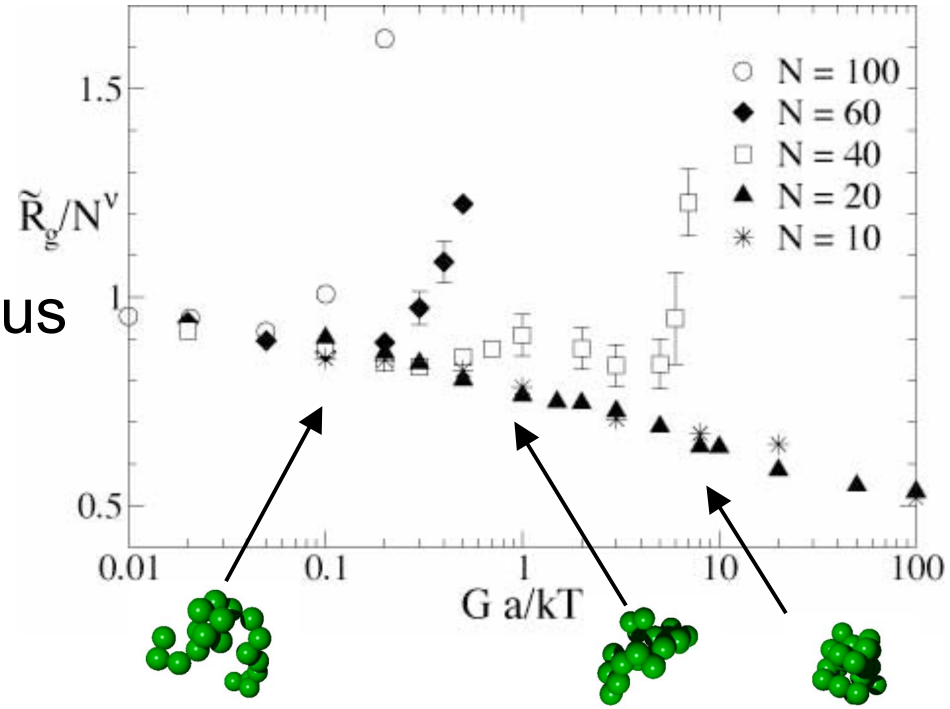
hydrodynamic drag -> internal recirculation with velocity $v \approx GN/\eta R$

-> recirculation time scale $\tau_{flow} \approx R/v \approx \eta R^2/GN$

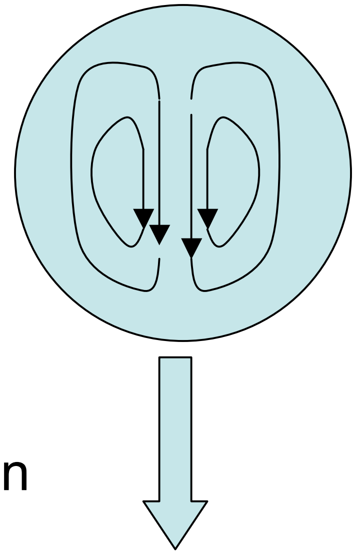
compare with coil relaxation time $\tau_R \approx \eta R^3/k_B T$

„scrambled/collapsed coil“ for $\tau_R > \tau_{flow}$ or $Ga/k_B T > N^{-2/3}$

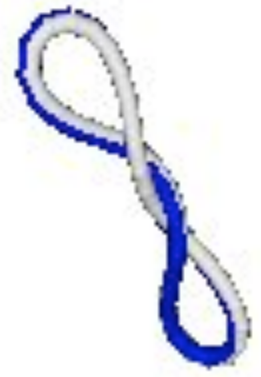
radius



sedimentation force



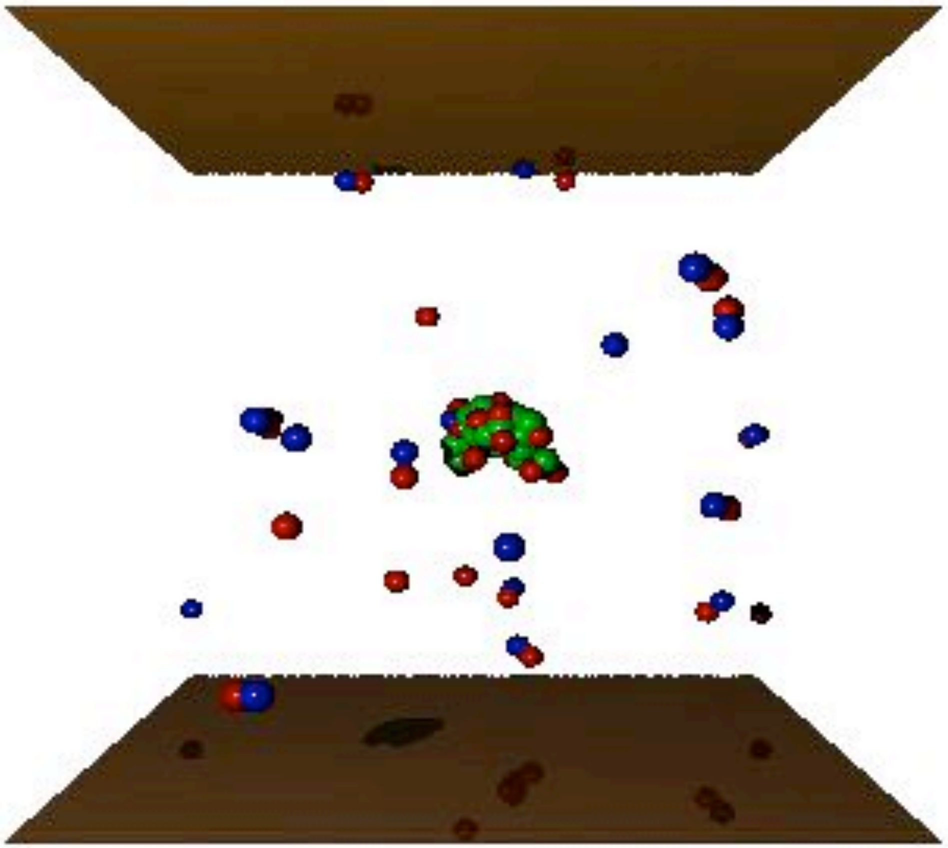
Sedimentation of twisted ring polymer (conserved linking number) Hirofumi Wada



Dynamics of plectoneme formation in ring polymer

Hirofumi Wada

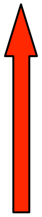
Electrophoresis of polyelectrolytes



20 monomers

40 counterions

20 coions



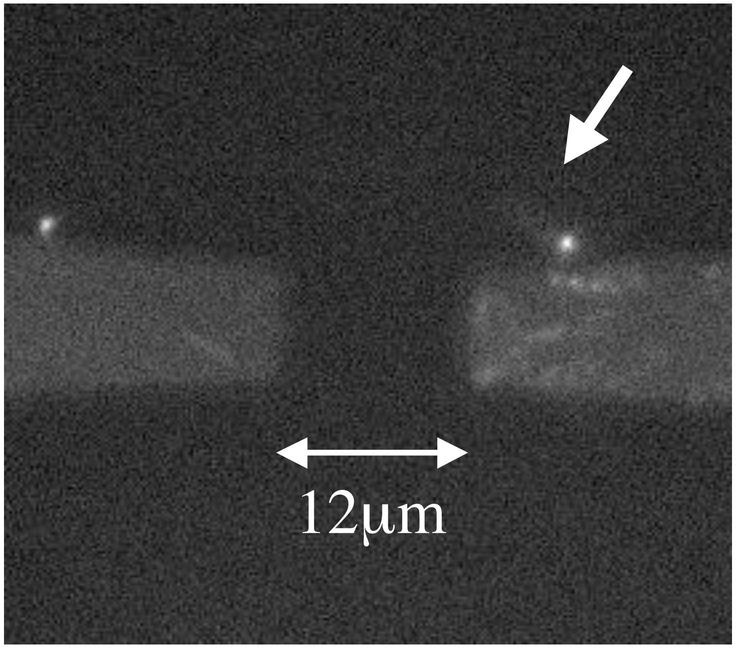
electric field,
camera moves
with polymer !

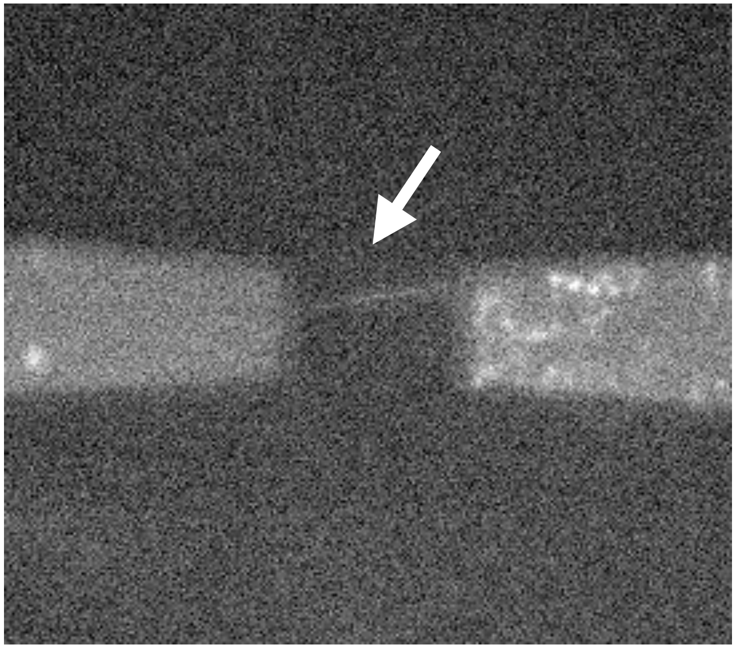
minimal image BC
strong coupling $\Xi = 20$

experimental observation of DNA stretching in fields

Beyer, Simmel (LMU)

4 Volts -> E = 3 x 10^5 V/m
DNA length 17µm
10mM HEPES, no added salt





DNA-molecules are typically stretched in free-solution electrophoresis experiments -> no length separation possible

Protein denaturation in shear flows

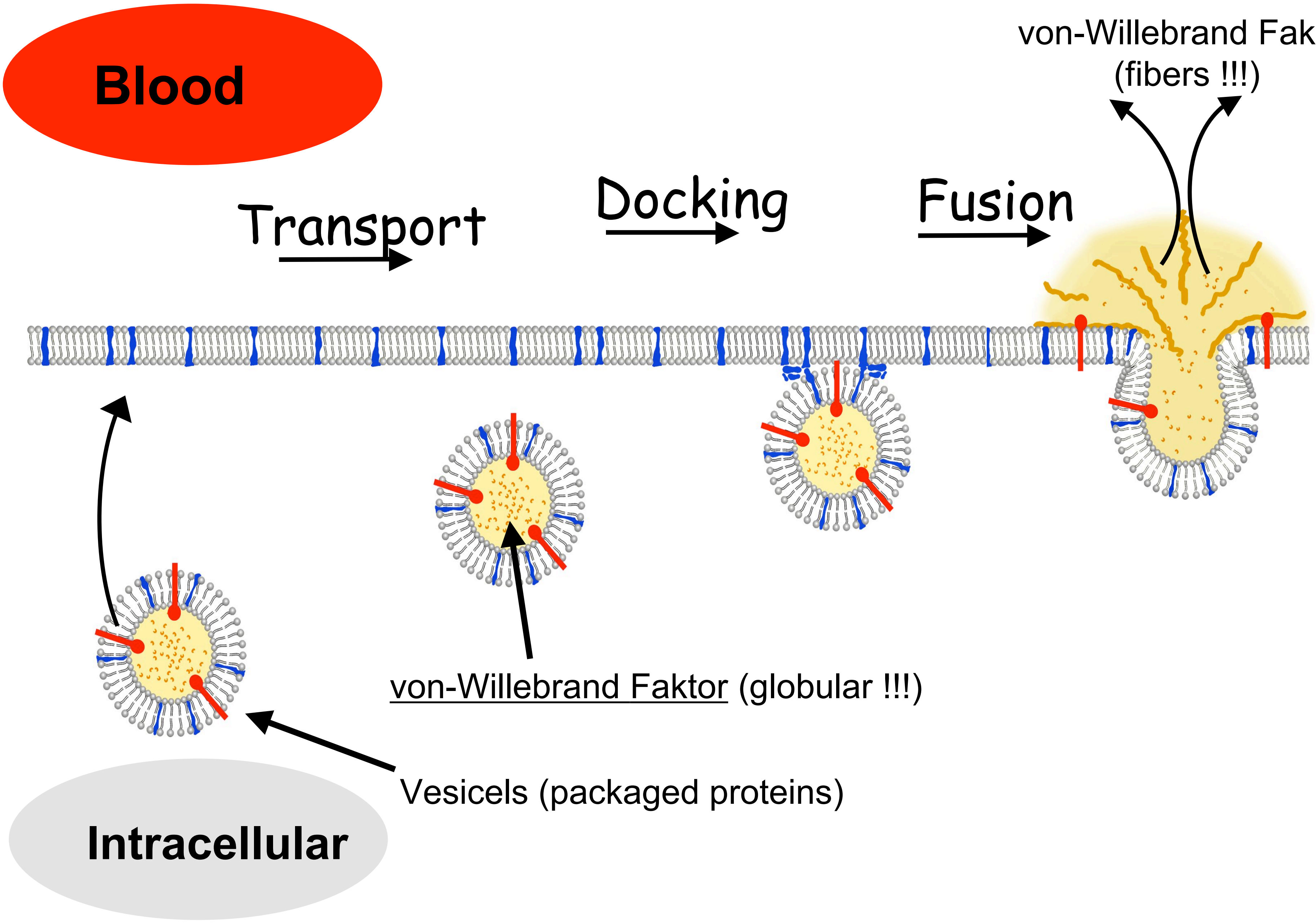
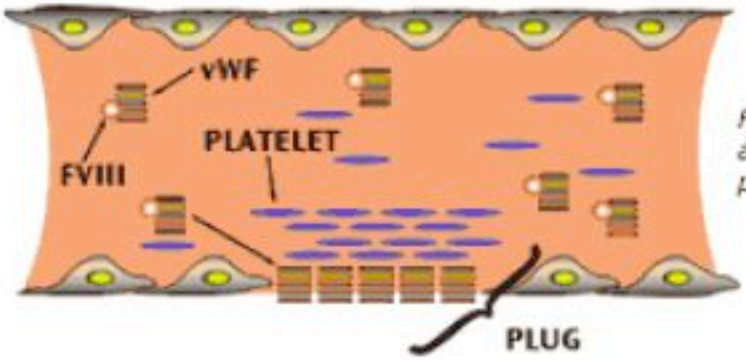


Figure 1. Normal Broken Blood Vessel



First, vWF proteins from the blood line up along the broken vessel wall and attract "sticky" platelets to form a plug.

Then the platelets attract strands of fibrin to strengthen the plug and form a clot. The clot helps stop the bleeding.

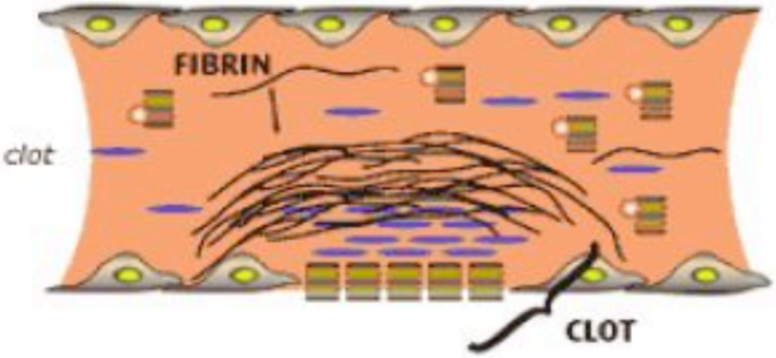
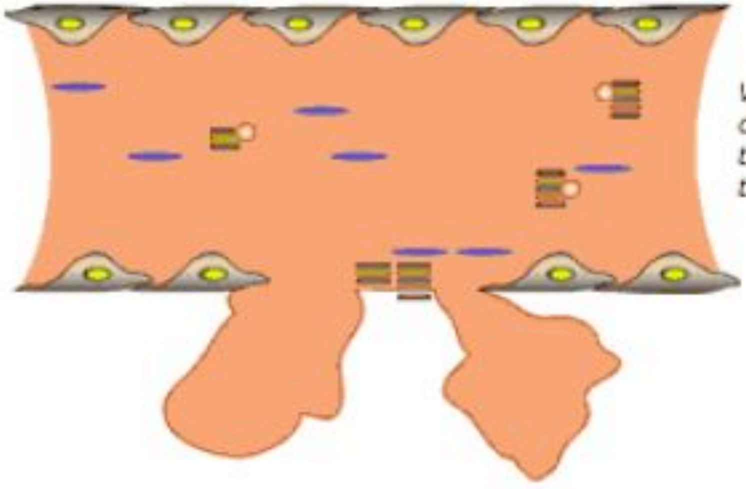


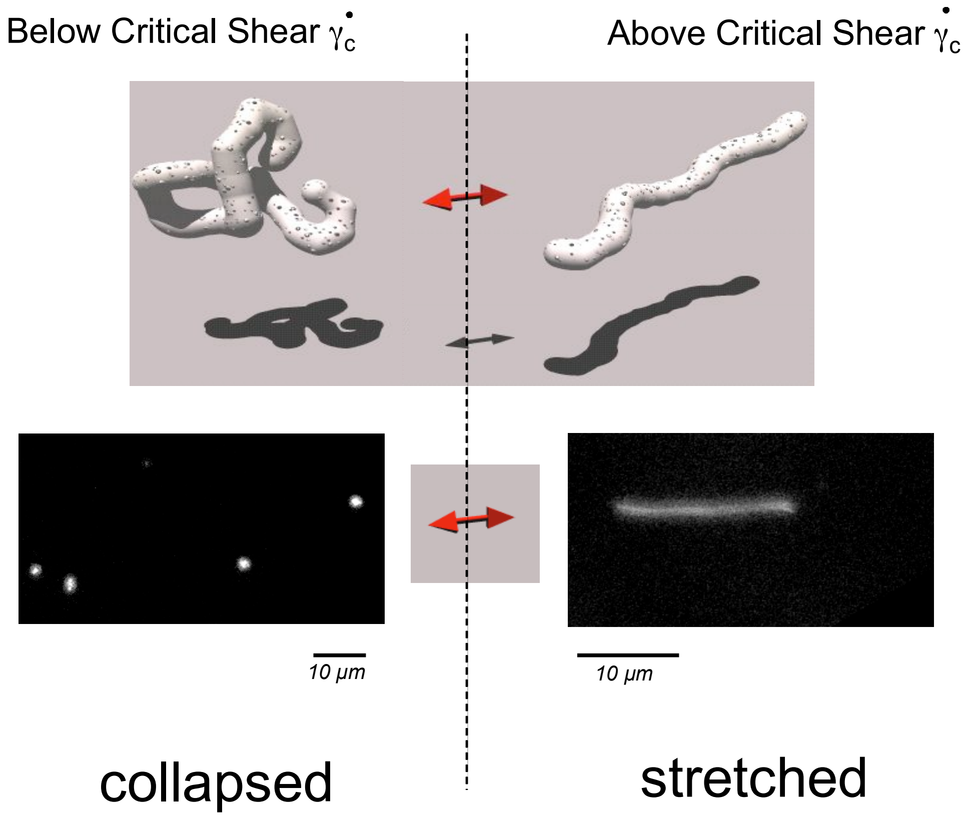
Figure 2. Broken Blood Vessel in vWD

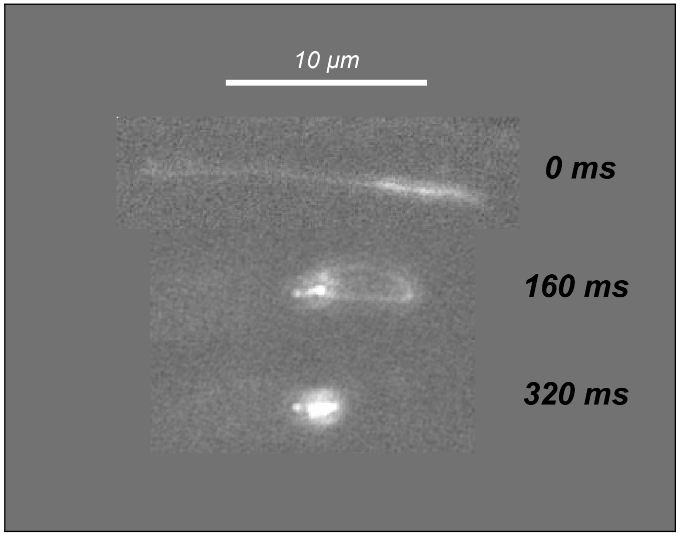


When a person has vWD, there isn't enough vWF or the vWF is damaged. The clot may take longer to form or not form properly, and bleeding make take longer to stop.

unfolding occurs also in bulk (without collagen substrate)

Schneider/Wixforth (Augsburg)



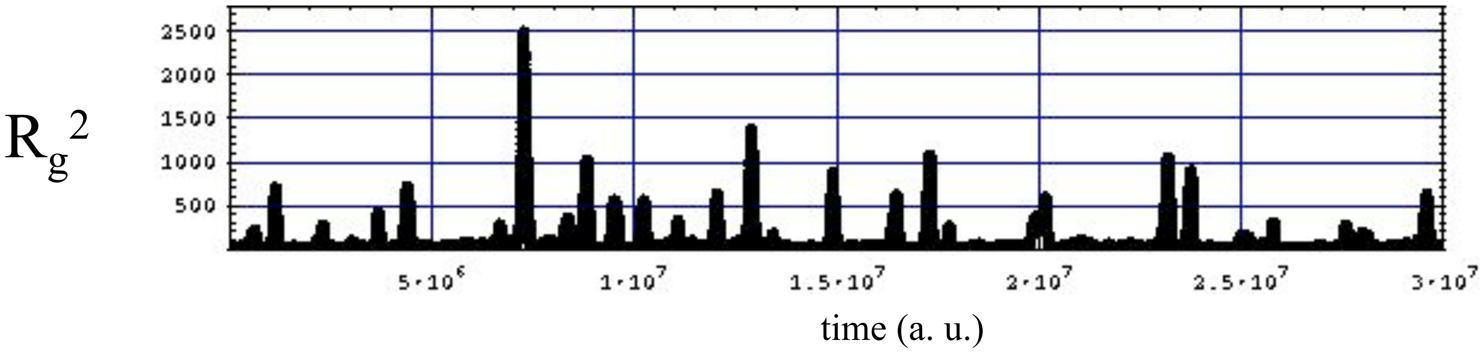


relaxation into globular state once shear is turned off

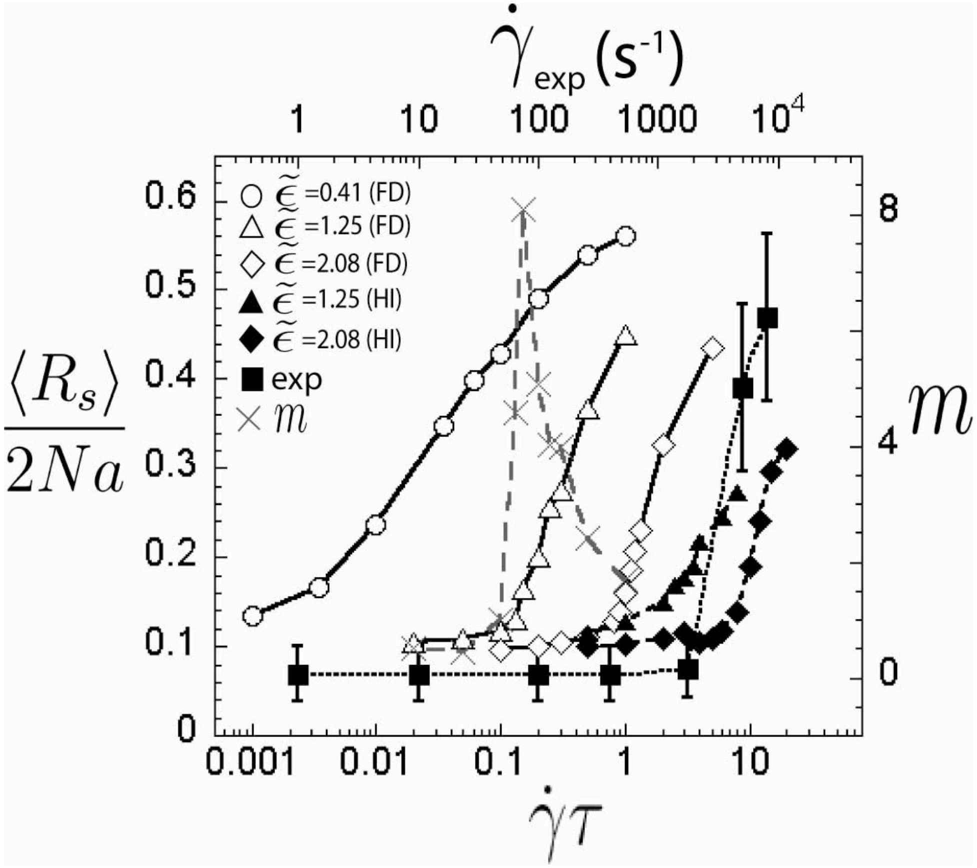
in shear, ε=2.5, γ=1.2

Alfredo Alexander-Katz

stretching dynamics



$\gamma \sim \gamma^*$



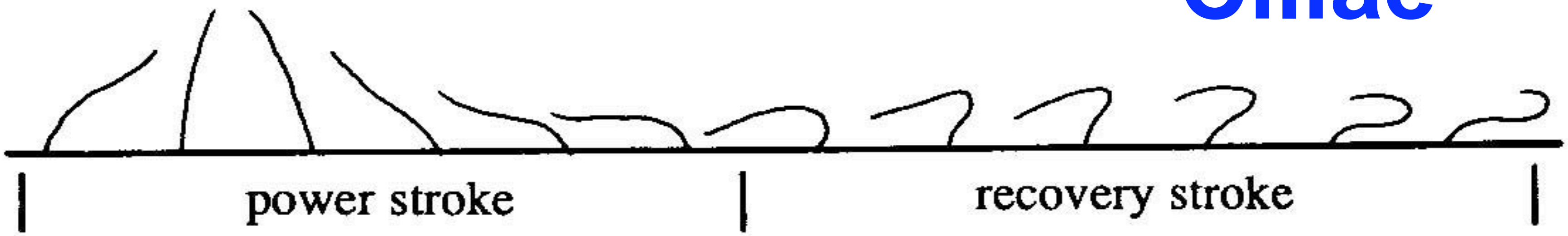
stretching response

unfolding becomes
abrupt for globular proteins
(in agreement with experiments)

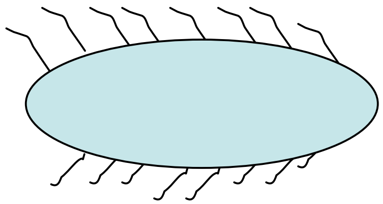
Propulsion with stiff polymers

produce shear with beating polymers

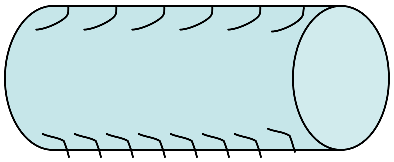
Ciliae



propulsion

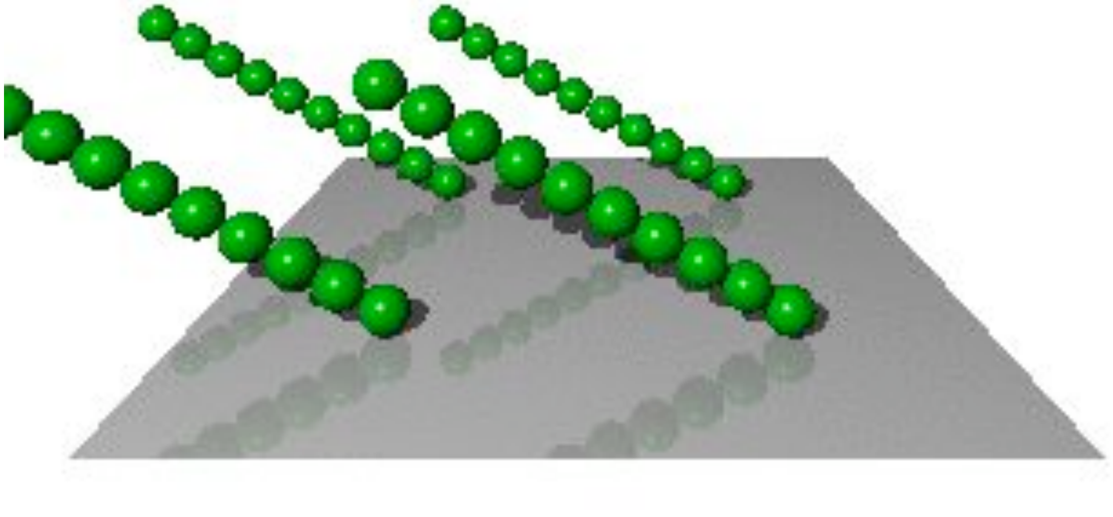


pumping



model polymer as isotropic elastic rod
apply asymmetric torque at the polymer base
-> measure net pumping velocity, efficiency, etc.

Yong-Woon Kim, RRN

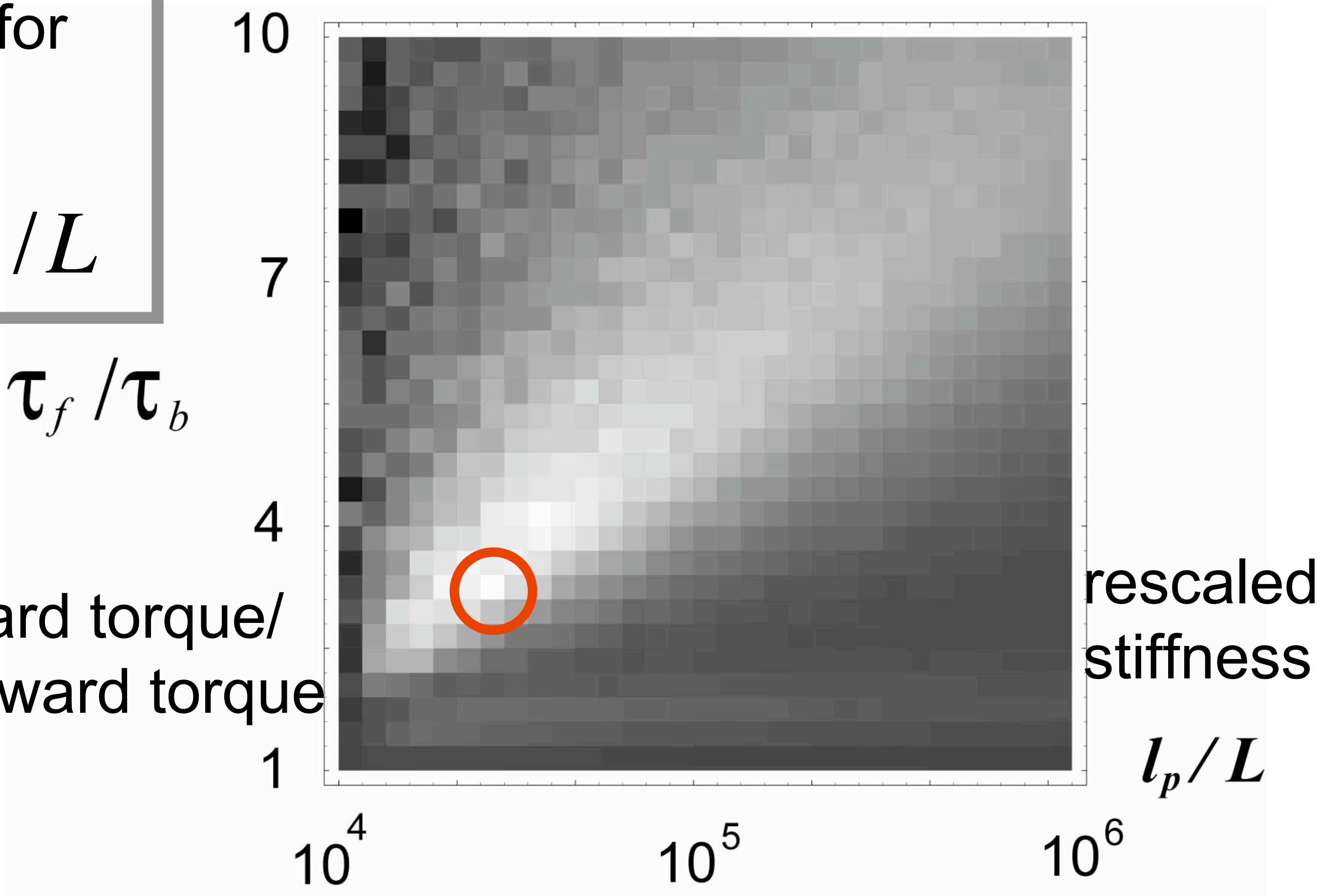


$$\text{pumping efficiency} = \frac{\text{net solvent velocity}}{\text{power input}}$$

1. condition:
threshold force for deformation:

$$\tau_f / k_B T \approx \ell_P / L$$

2. Condition: asymmetry

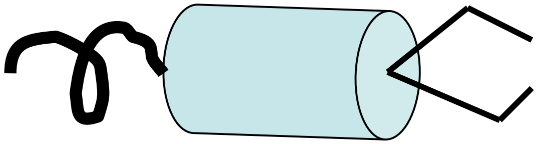


Symmetric motion: no net pumping

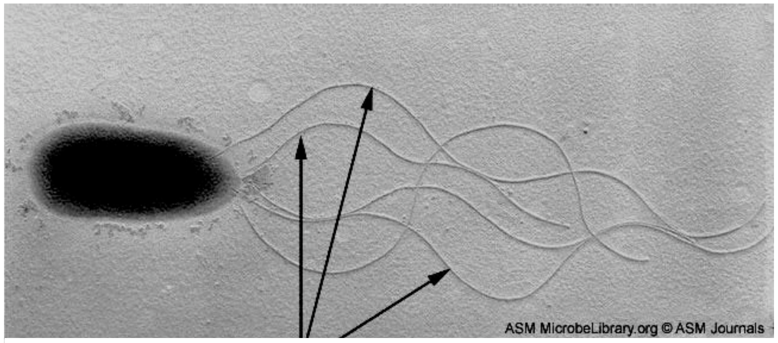
No elasticity: no net pumping (since reciprocal motion…)

propulsion with single rotating polymers

goal:
moving nanomachines



- Bacteria



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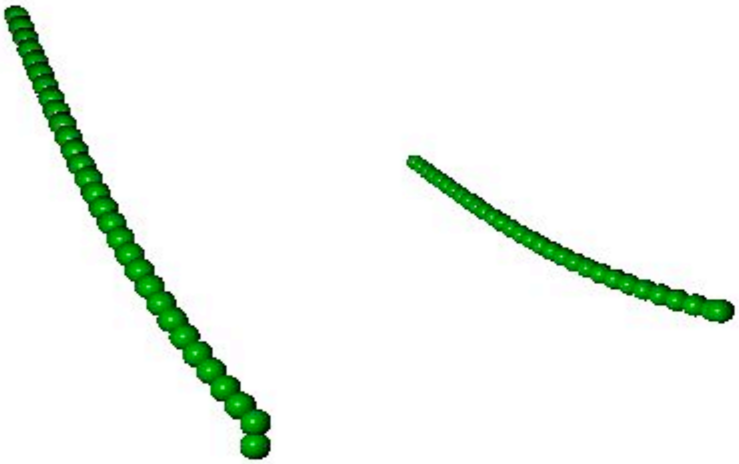
Pseudomonas Putida

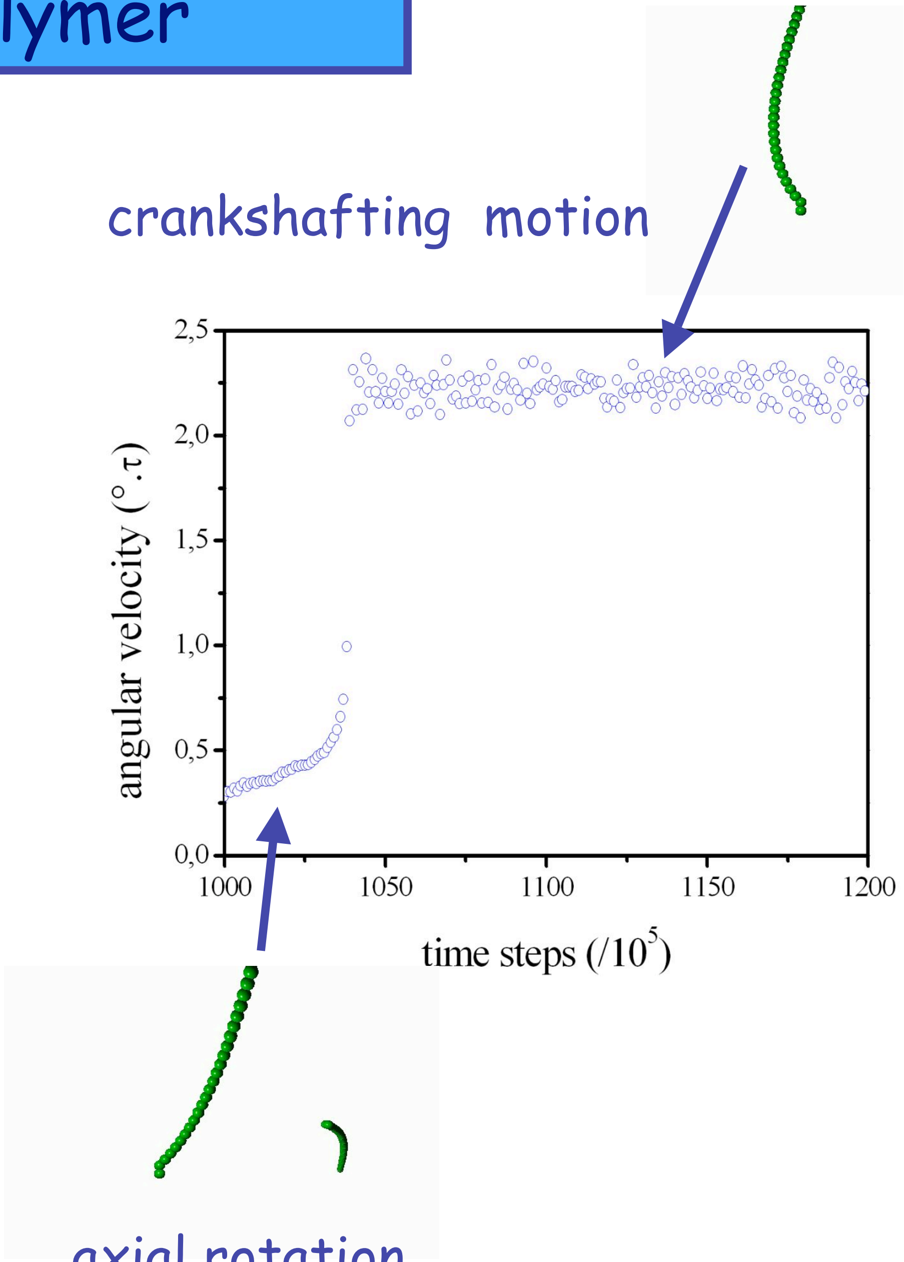
problem: - need helical polymer,
- rotational sense determines thrust direction

question: - propulsion possible with straight rotating polymers?

Dynamical transition for rotating straight flexible polymer

Manoel Manghi/ RRN




crankshafting motion

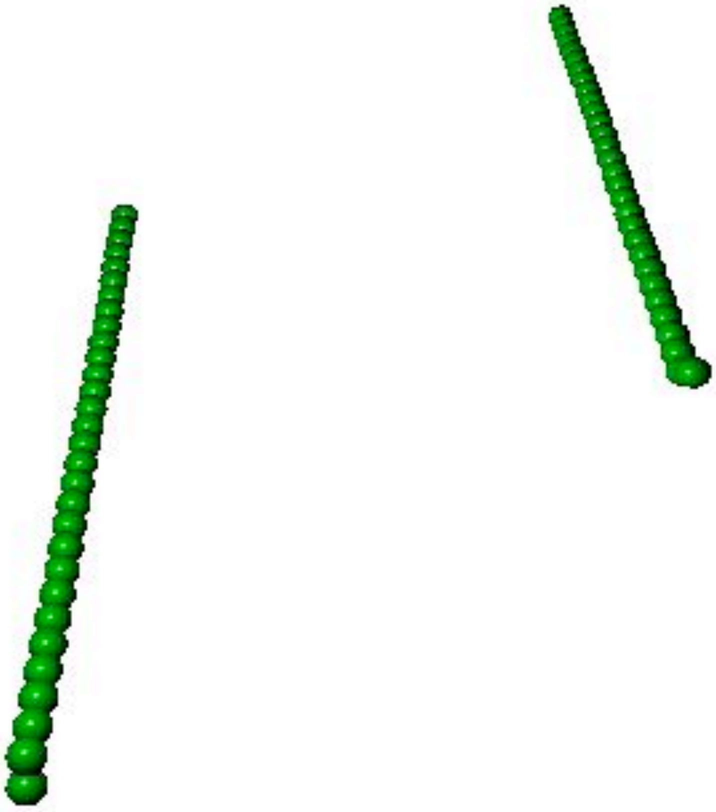
axial rotation

Torque = 4-5 kT/rad

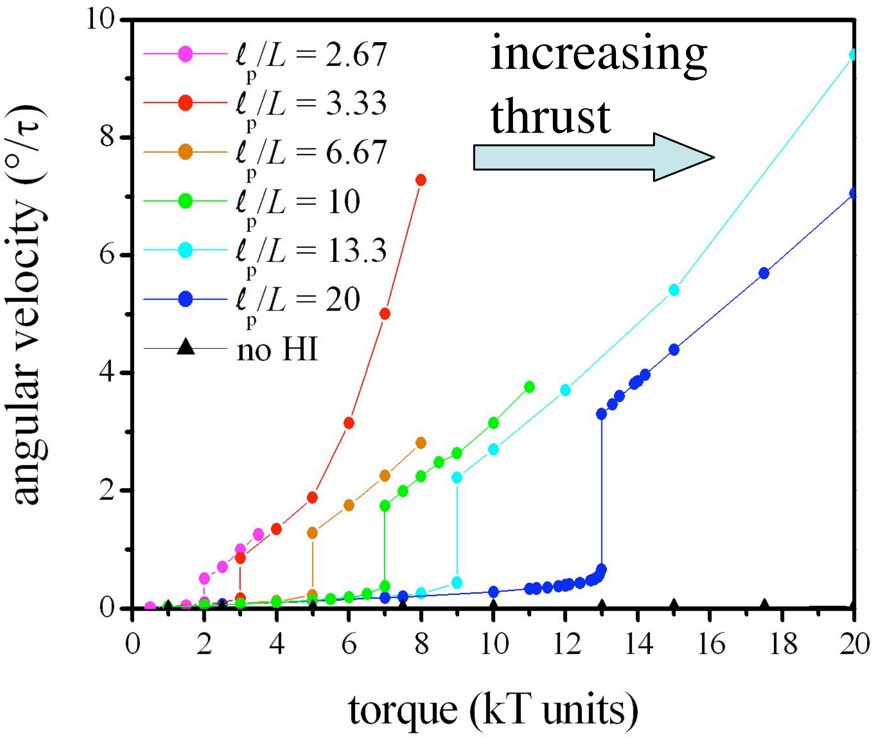
ℓ_p = 6.7 L

N = 30

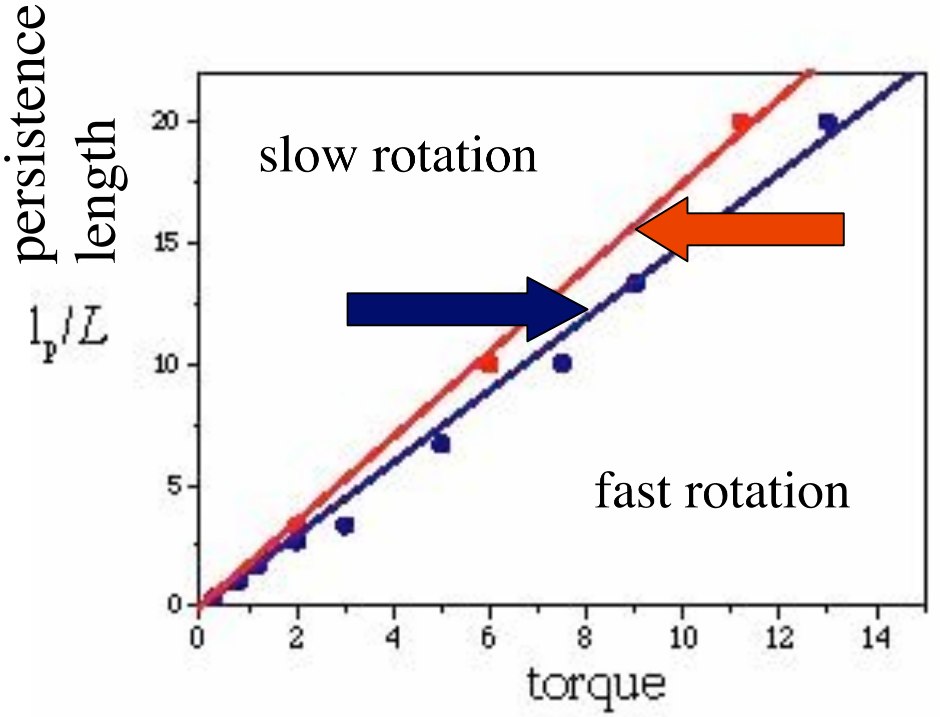
flexible polymer , l_P=L/3
effects of thermal fluctuations?



discontinuous non-eq. shape transition



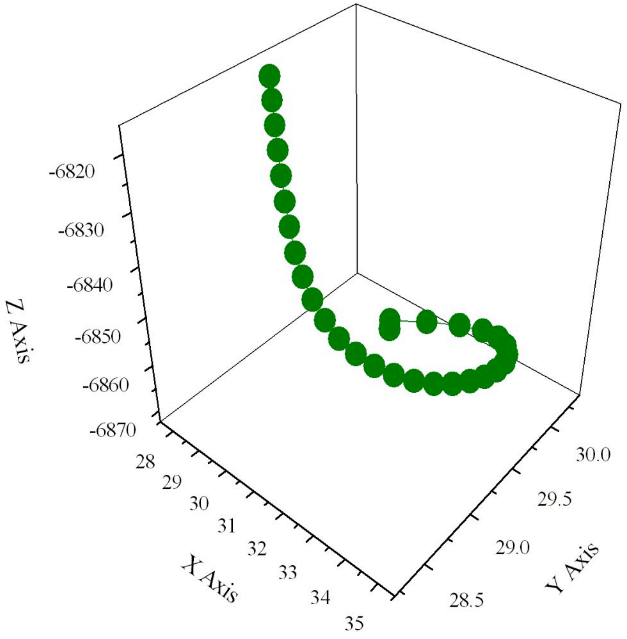
hysteresis



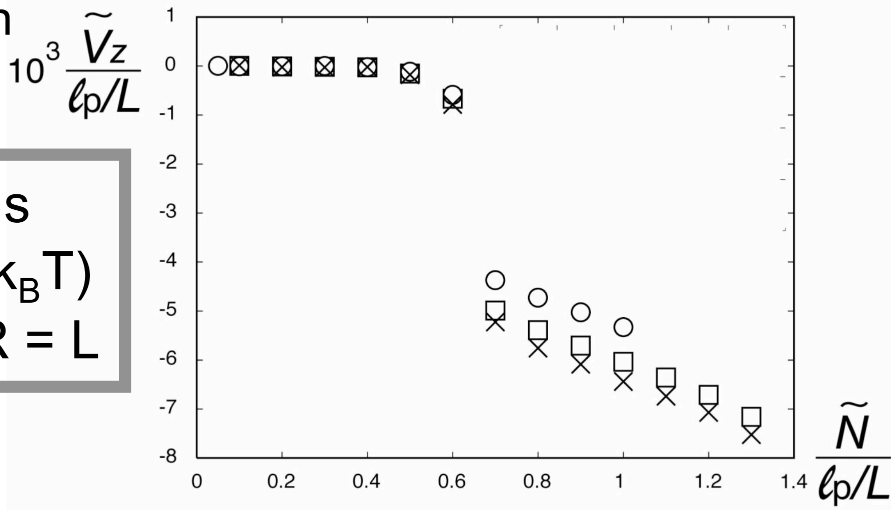
Propulsion due to breaking of time-reversal invariance of motion

thrust direction independent of rotational sense !!

---> **nano-force-rectifyer**



Propulsion velocity



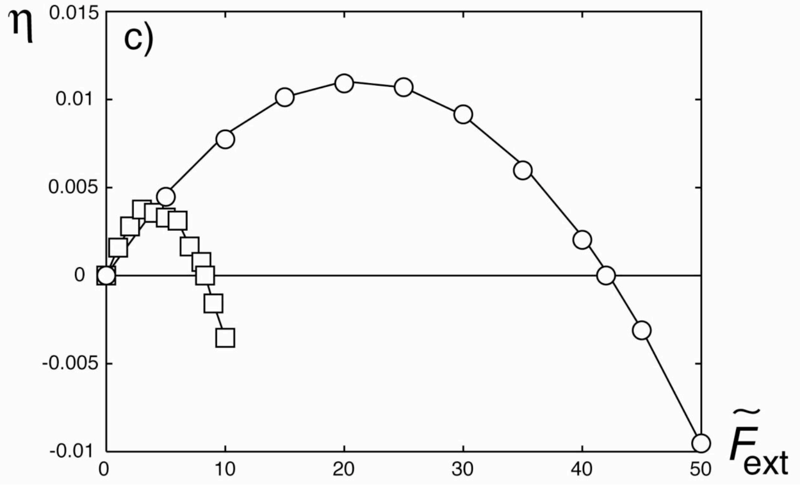
Rescaled applied torque

bending radius

$1/R = N / (\ell k_B T)$

transition at R = L

Propulsion efficiency



Loading force

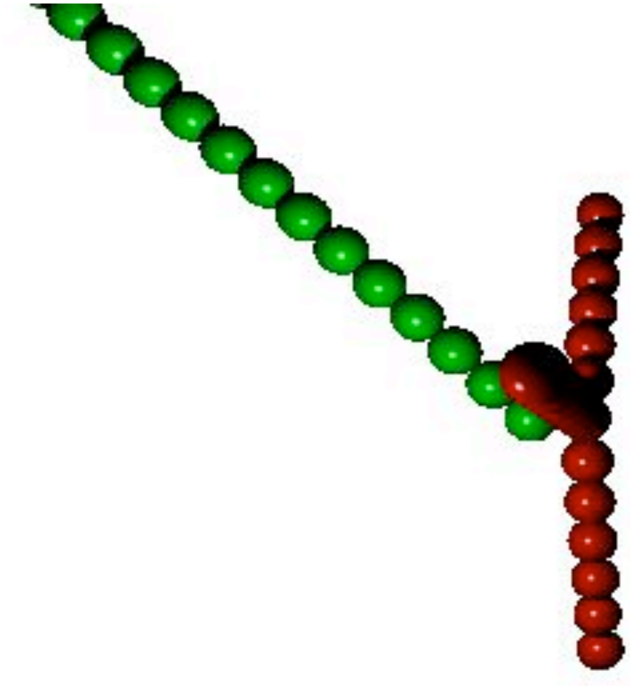
$$\eta = \frac{\text{propulsion power}}{\text{rotation power}}$$

efficiency low (but not worse than bacterial flagellae)

Flagellum with a base: total force and torque must be zero

→rotation leads to counterrotation

→trajectories are complex



Hirofumi Wada

first form helix (difficult!):

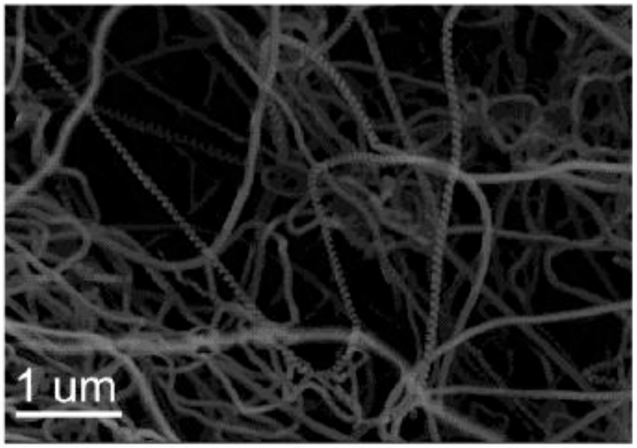
then rotate, slowly

quickly
(periodic twist-stretch conversion)

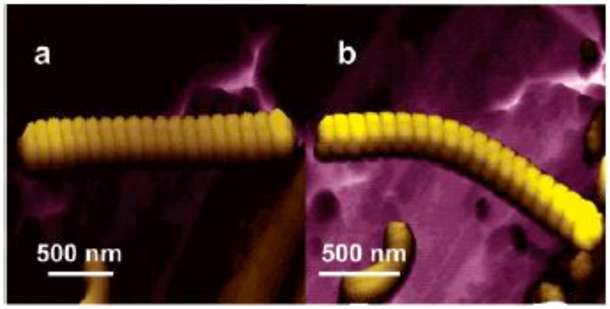
-shape (polymorphism??), bundling, efficiency……

pulling on helical nanosprings

Hirofumi Wada (JSPS-fellow) & RRN



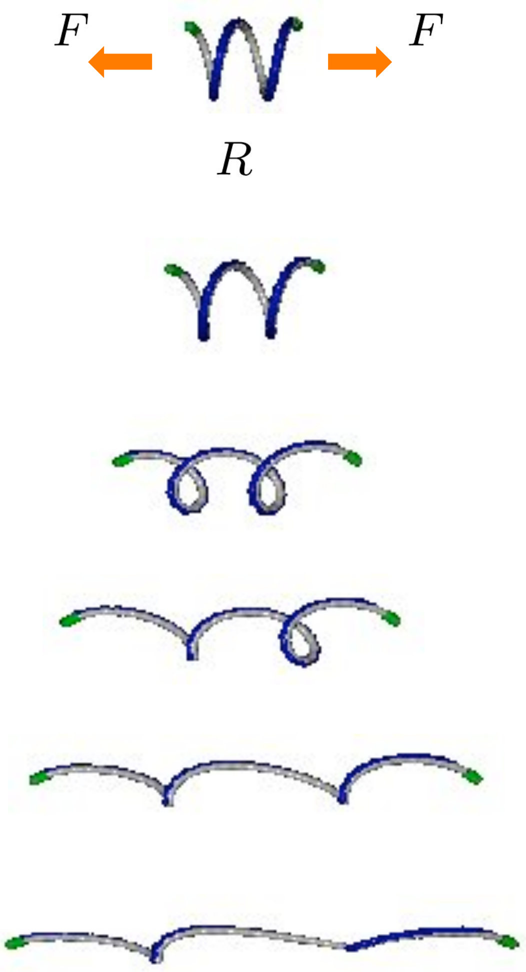
SEM characterization of as-synthesized silicon oxide nanowires



AFM manipulation of a helical silica nanospring

Hai-Feng Zhang *et al.* Nano Lett. **3** 577 (2003)

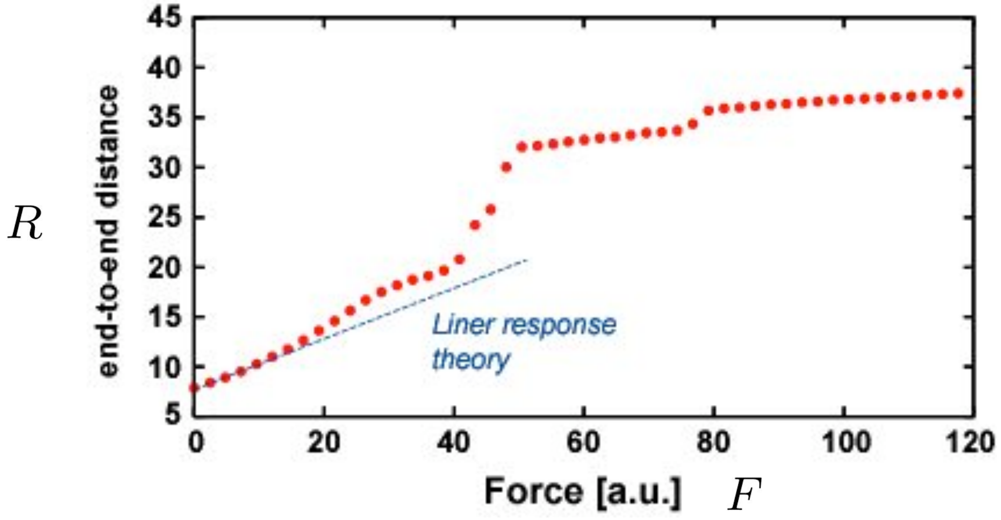
pulling on a nanospring



Linear response for small pulling force

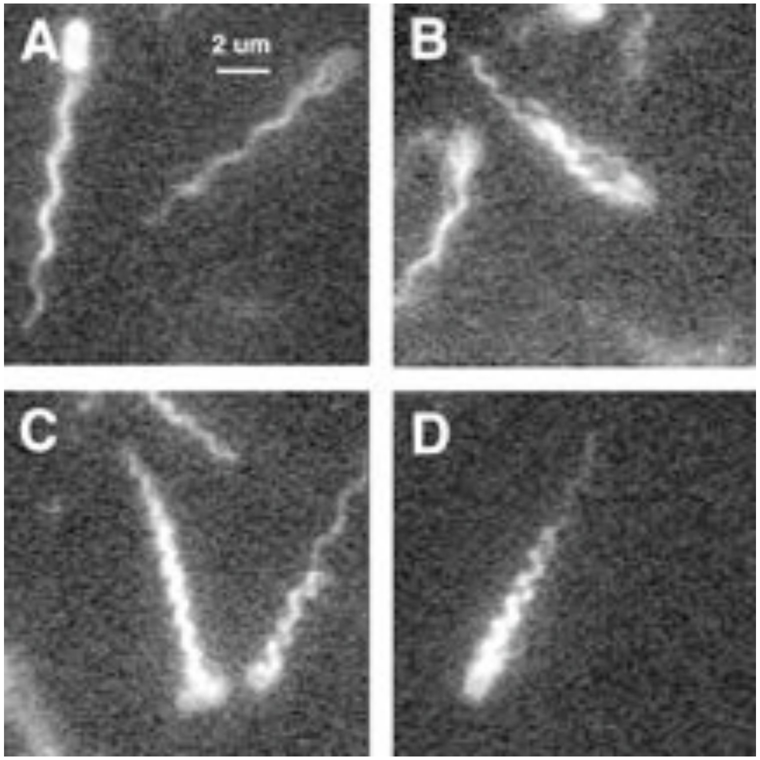
$$F \approx K_{sp}(R - R_0)$$

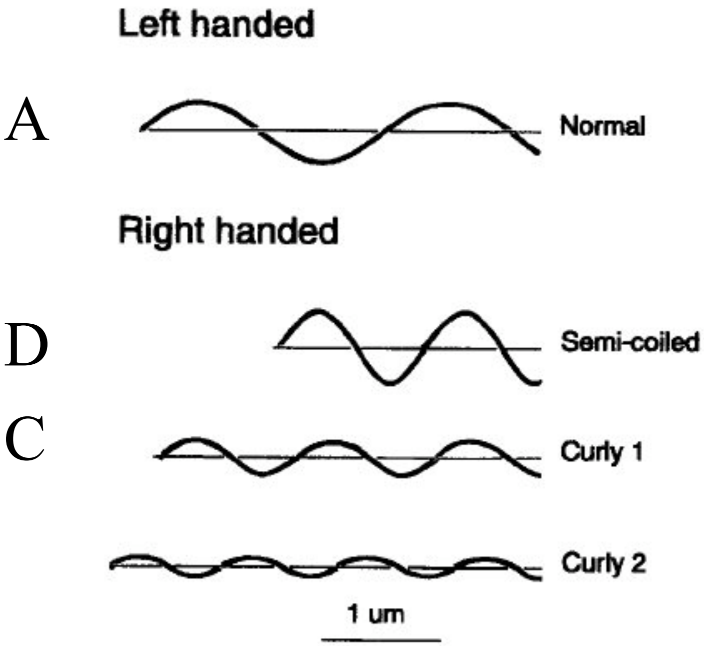
$$K_{sp} = \frac{\Omega_0^2}{L}\left[4A\beta^2 + C(1-\beta^2)^2\right]$$



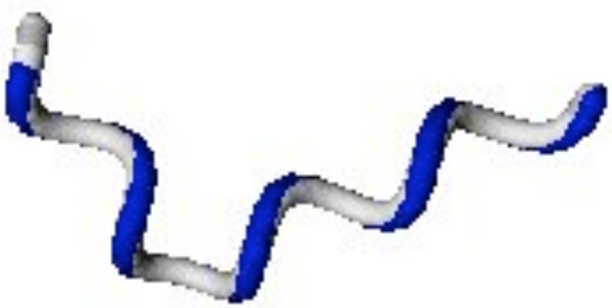
Force-extension curve reveals stretching instability of a helical nanospring.

Polymorphic transformations of flagellae as function of rotational sense and frequency





Dynamic conversion of bistable helix



design of simple propulsion devices
with stiff polymers
leads (naturally) to biomimetic structures ….