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**

\[ \eta \Delta \vec{v} \left( \vec{r} \right) - \nabla p = \rho \left( \vec{v} \cdot \nabla \right) \vec{v} \]

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**.

<table>
<thead>
<tr>
<th>Human</th>
<th>Bacterium</th>
<th>Sinking cylinder</th>
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</table>
| \[H_2O: \quad \eta = 0.001 \text{ Pa s;} \]
| \[\rho = 1000 \text{ kg/m}^3\]
| \[v = 1 \text{ m/s}\]
| \[l = 1 \text{ m}\]
| \[\text{Re} = 10^6\]
| \[v = 10^{-5} \text{ m/s}\]
| \[l = 1 \mu\]
| \[\rightarrow \text{Re} = 10^{-5}\]
| \[v \sim 10^{-7} \text{ m/s}\]
| \[l = 1 \mu\]
| \[\rightarrow \text{Re} = 10^{-7}\] |
flow-field due to point-force at origin:
\[ u^\alpha(r) = H^{\alpha\beta}(r) f^\beta \quad \alpha,\beta = 1,2,3 \]
\[ H^{\alpha\beta}(r) = \frac{1}{8\pi\eta r} \left[ \delta_{\alpha\beta} + \hat{r}^\alpha \hat{r}^\beta \right] \]
(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:

\[
\dot{m \vec{r}}_j(t) \bar{\mu}_{ij} + \dot{r}_i(t) = \bar{\mu}_{ij} f_j(t) + \xi_i(t)
\]

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

Random force \( \langle \xi_i(t) \xi_j(t') \rangle = 6 \bar{\mu}_{ij} k_B T \delta(t - t') \)

Mobility matrix:

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

self mobility:

\( \mu_0 = (6\pi R \eta)^{-1} \) hydrodyn. interact.

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

\[
\frac{\partial W}{\partial t} = \sum_{i,j} \frac{\partial}{\partial r_i} \left[ D_{ij} \frac{\partial W}{\partial r_j} - \bar{\mu}_{ij} f_j W \right] \quad \text{with solution: } \quad W \approx e^{-U / k_B T}
\]

Velocity of \( i \)-th particle:

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\]
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 $v \approx GN^{1-\nu}$
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 $Ga/k_B T > N^{-2/3}$
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 -> $E = 3 \times 10^5$ V/m
DNA length 17$\mu$m
10mM HEPES, no added salt

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

Blood

Transport

Docking

Fusion

von-Willebrand Faktor (fibers !!!)

Von-Willebrand Faktor (globular !!!)

Intracellular

Vesicles (packaged proteins)
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, $\varepsilon=2.5, \gamma=1.2$  

Alfredo Alexander-Katz
stretching dynamics

\[ \gamma \sim \gamma^* \]

unfolding becomes abrupt for globular proteins (in agreement with experiments)
Propulsion with stiff polymers
Cilia produce shear with beating polymers

- **Ciliae**
  - power stroke
  - recovery stroke

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

1. condition: threshold force for deformation:
\[ \frac{\tau_f}{k_B T} \approx \frac{\ell_p}{L} \]

2. Condition: asymmetry

Threshold force for deformation:
\[ \frac{\tau_f}{\tau_b} \]

Ratio: forward torque/ backward torque

Symmetric motion: no net pumping
No elasticity: no net pumping (since reciprocal motion...)

rescaled stiffness

10^4 10^5 10^6

\( l_p / L \)
propulsion with single rotating polymers

- need helical polymer,
- rotational sense determines thrust direction

question: - propulsion possible with straight rotating polymers?

Pseudomonas Putida

• Bacteria

goal: moving nanomachines
Dynamical transition for rotating straight flexible polymer

Torque = 4-5 kT/rad
\( \ell_p = 6.7 \) L
N = 30

Manoel Manghi/RRN

crankshafting motion

axial rotation

angular velocity (°/τ)

time steps (/10^5)
flexible polymer, \( l_p = L/3 \)
effects of thermal fluctuations?
discontinuous non-eq. shape transition

hysteresis

increasing thrust

slow rotation

fast rotation
Propulsion due to breaking of time-reversal invariance of motion thrust direction independent of rotational sense!!
----> nano-force-rectifier

\[ \frac{1}{R} = \frac{N}{(\ell k_B T)} \]

transition at \( R = L \)

\[ \eta = \frac{\text{propulsion power}}{\text{rotation power}} \]

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
pulling on a nanospring

Linear response for small pulling force

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

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

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

![Diagram showing the stretching of a helical nanospring under force, with equations and a graph depicting force-extension behavior.](image)
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 ....