XXVII Fluid Mechanics Conference

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Flow of DNA Chains in Molecular and Microfluidic Systems

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DNA

DNA is a long (**2 meter x 2nm**) flexible polymer that stores, transmits, and executes the instructions needed to build and maintain life. It contains over **6 billion base pairs**.

In solution, it behaves like a tiny, fluctuating thread influenced by fluid forces, thermal motion, and confinement.

Inside a cell due to its vast size, extreme flexibility, and sequence-dependent structure **kept in a very small volume of the nucleus** makes DNA a challenging system to model in <u>soft matter physics</u> and <u>polymer physics</u>.

All-atom Molecular Dynamics computational methods for DNA have limited applicability (0.1s, 10^9 base pairs).

DNA Dynamics Study

- Advances in molecular biology enable the direct, real-time visualization of individual DNA molecules.
- The DNA molecules are tethered at one end to a microscopic polystyrene bead using optical tweezers.
- Fluid flow could stretch the tethered DNA molecule to its full extension, **allowing the study of the stretching and relaxation kinetics of single DNA molecules in real-time!**

MECHANICS OF DNA

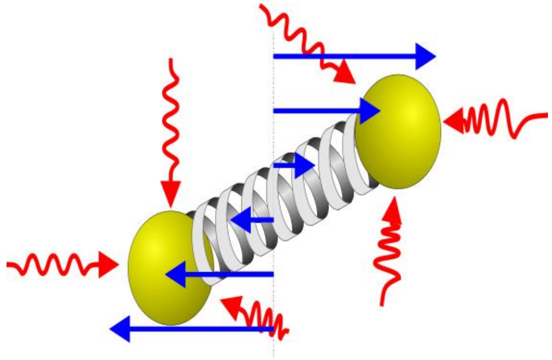
The *blob* model, the chain of segments.

The conditions of existence of jumps in the thermal motion of macromolecules of complex architecture.

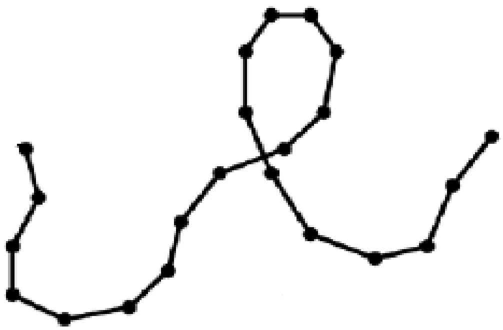
The tube model, explaining the essentially one-dimensional mobility of long polymer chains.

Entangled polymers are characterized by an effective internal scale, commonly known as *the length of macromolecule between adjacent entanglements*

Computer modeling



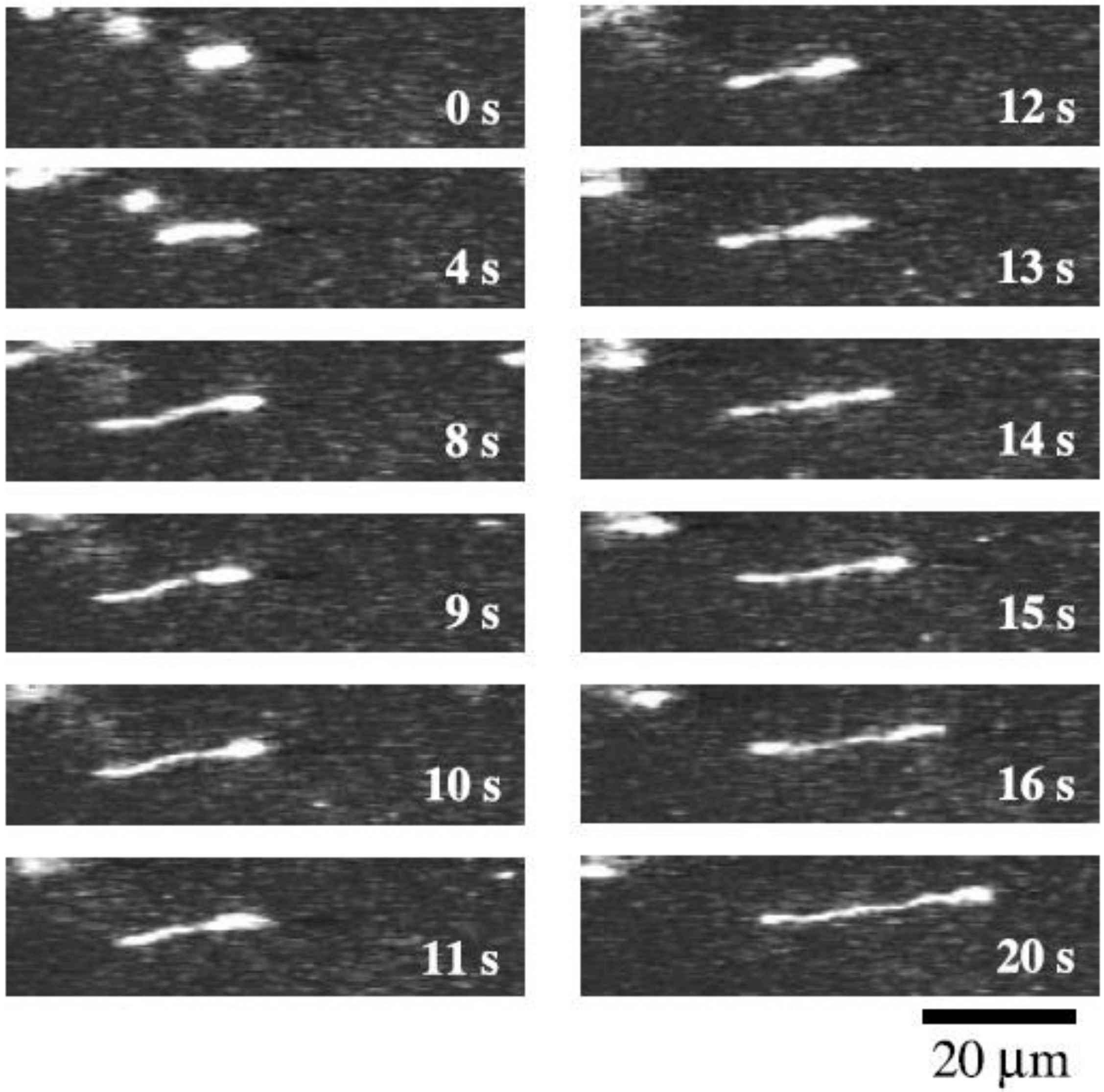
Dumbbell Model



Worm-Like Chain

DNA in flow is a nonlinear, stochastic elastic filament whose dynamics emerge from competition between hydrodynamics, entropy, and thermal noise.

Molecular Stretching of DNA

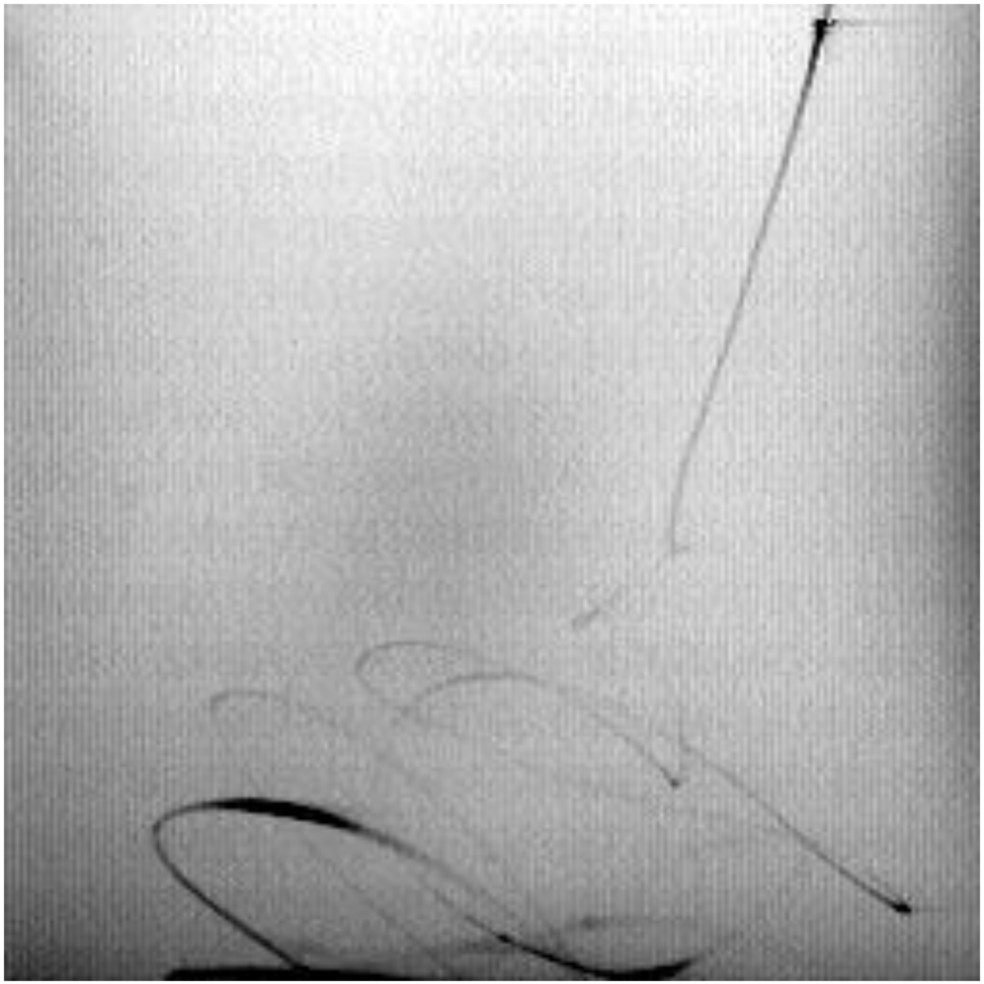


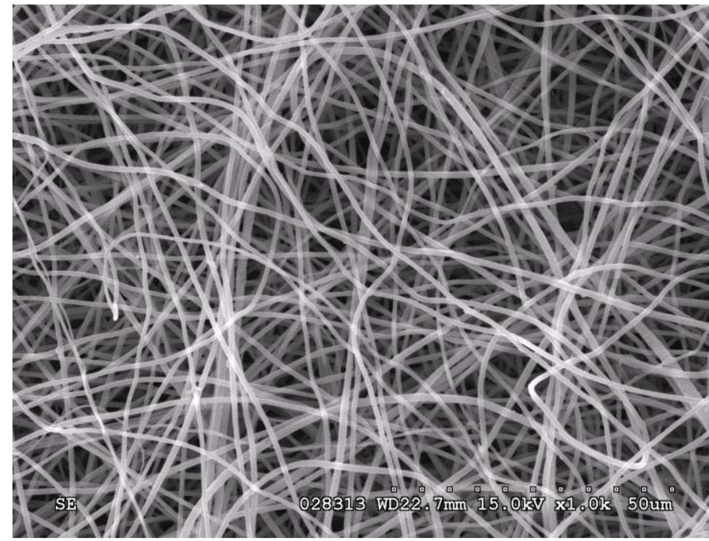
Experimental: Noritada Kaji, Masanori Ueda, and Yoshinobu Baba,

The molecular motion of a long DNA in agarose gel

Our micro scale experimental model

Fluorescent fibers obtained by electrospinning



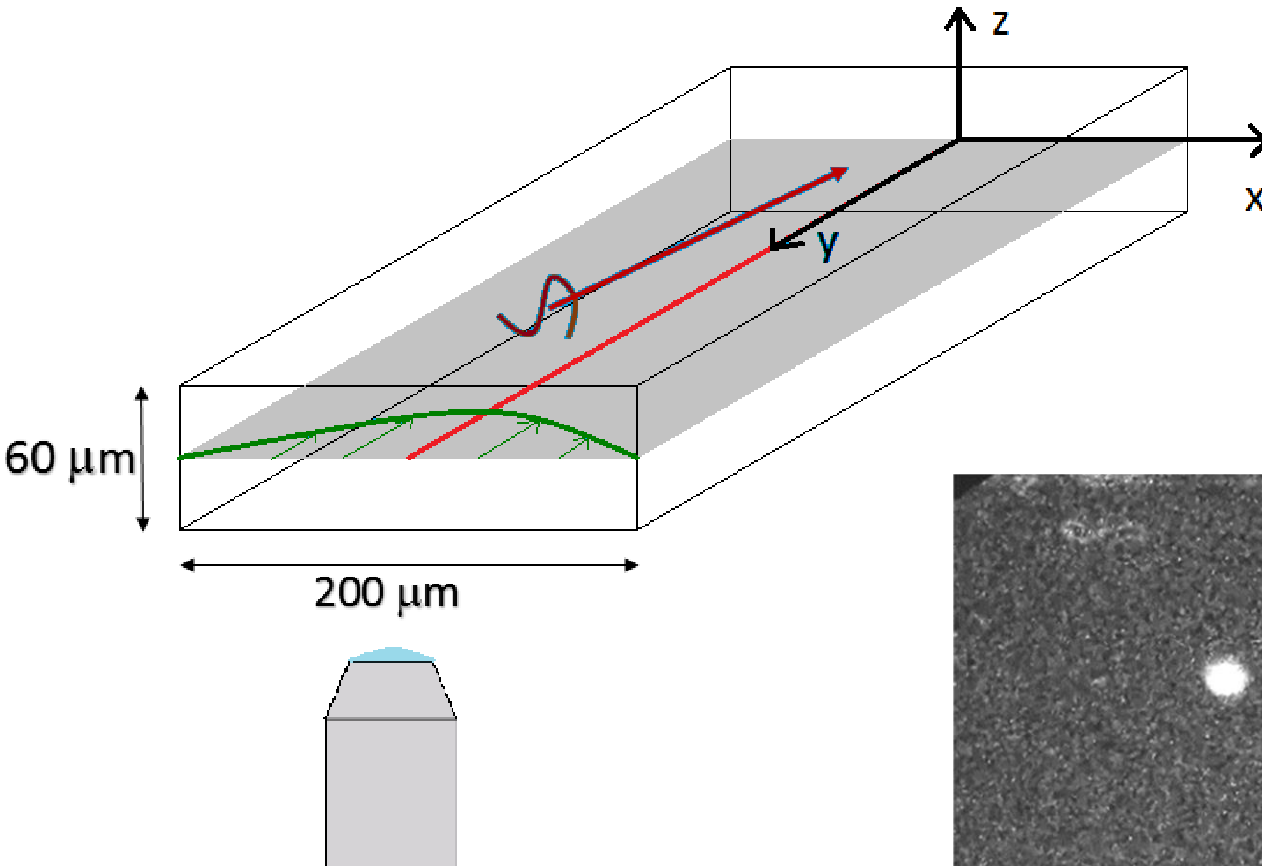


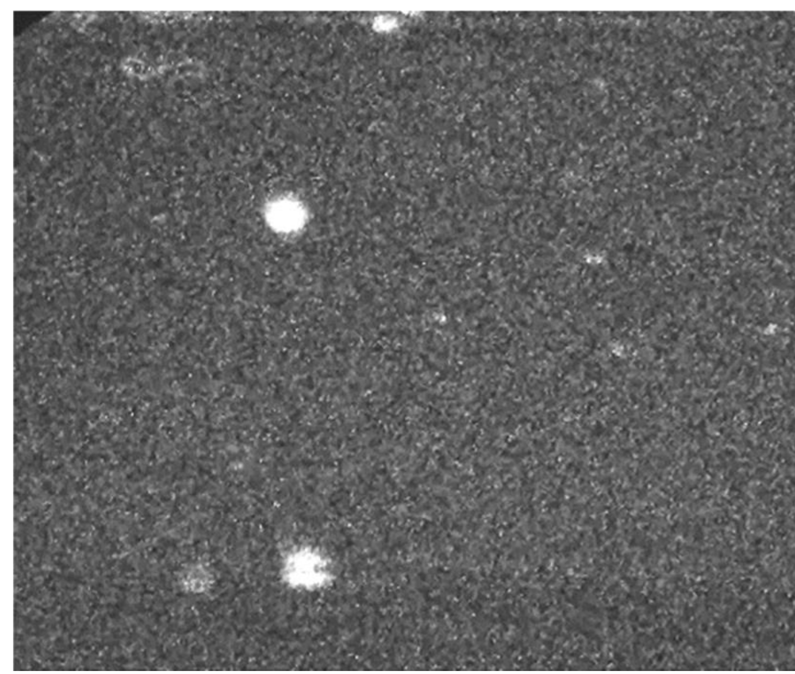
Target:

Suspension of short (1mm) x 500nm in diameter fibers

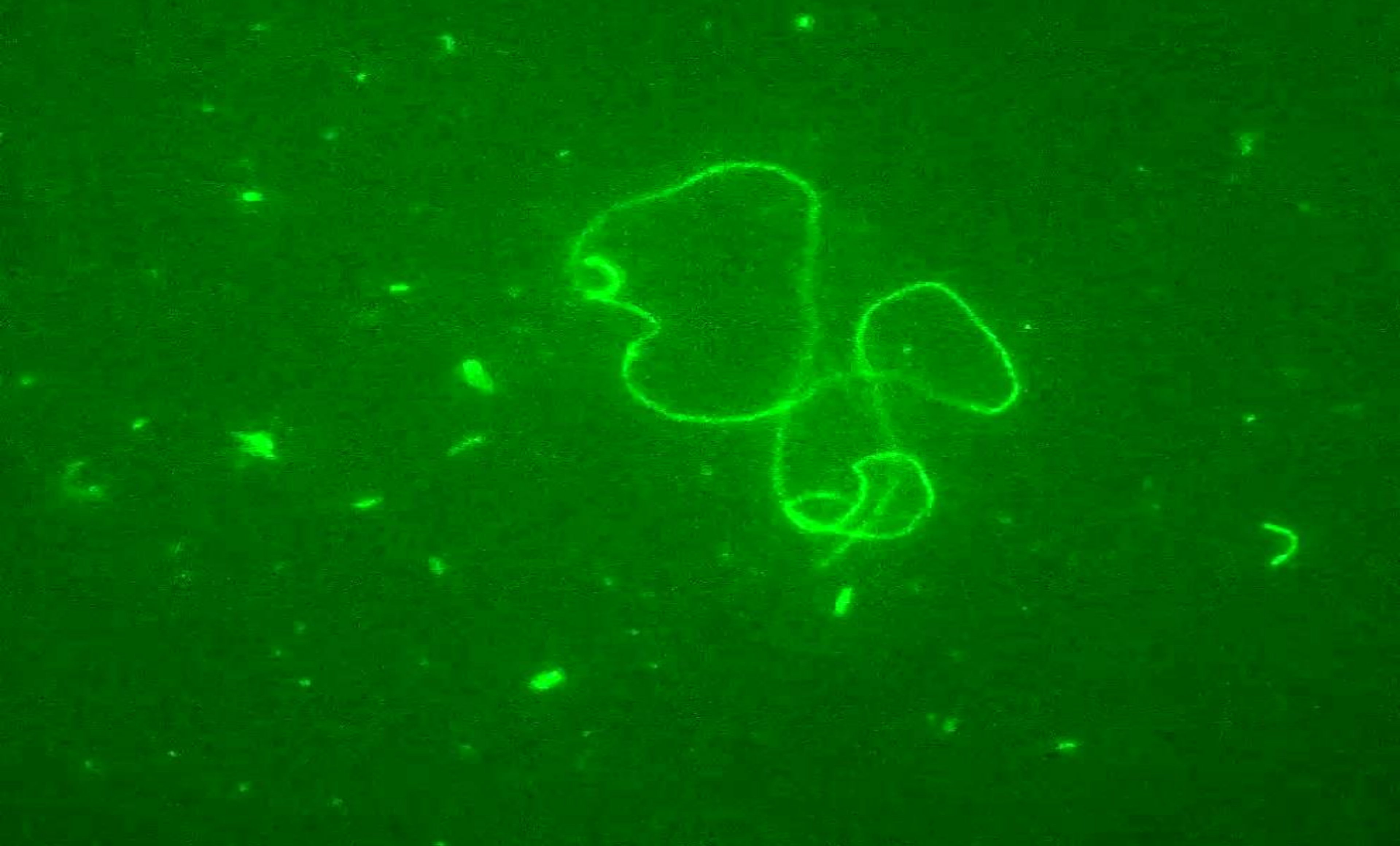
Water-insoluble PLLA fibers with Rhodamine A

Hydrogel filaments in flow





Brownian motion of highly deformable filaments



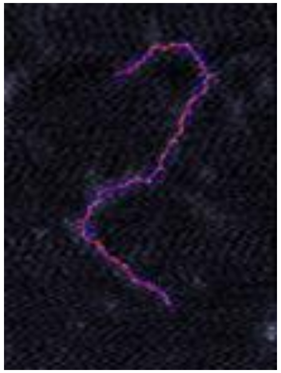
Typical parameters obtained for Brownian motion of hydrogel filament

Contour length: 15.6 μm
Persistence length: 598 μm

Experimental diffusion coefficients:
$D_a = 0.266\ \mu m^2$
$D_b = 0.070\ \mu m^2$
$D_{rot} = 0.0023\ rad^2$

Hydrogel microfilaments as an experimental model of elongated biomolecules

DNA



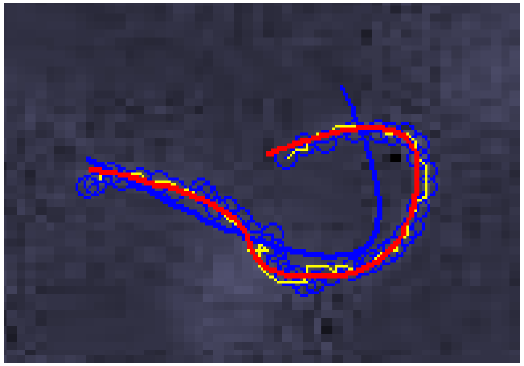
Persistence length: 118 nm
Contour length: 1379 nm
(AFM topography)

$$\frac{Lp}{L}$$

0,0855

0,0997

Hydrogel filament

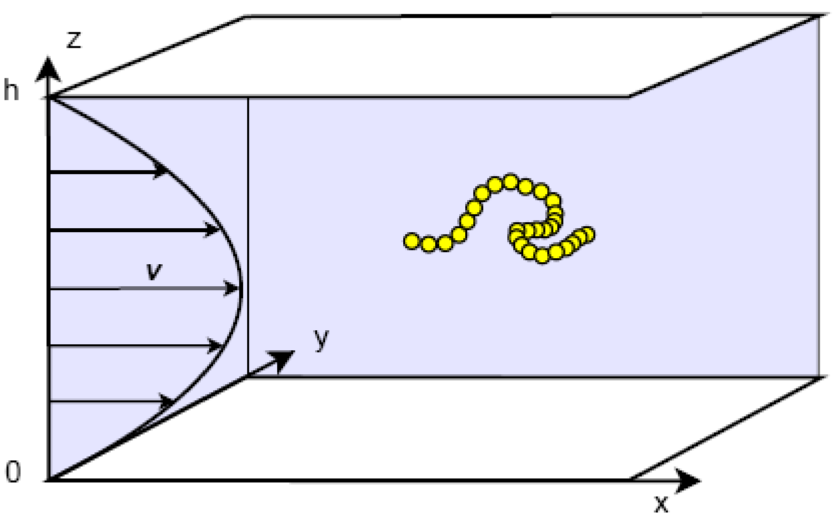


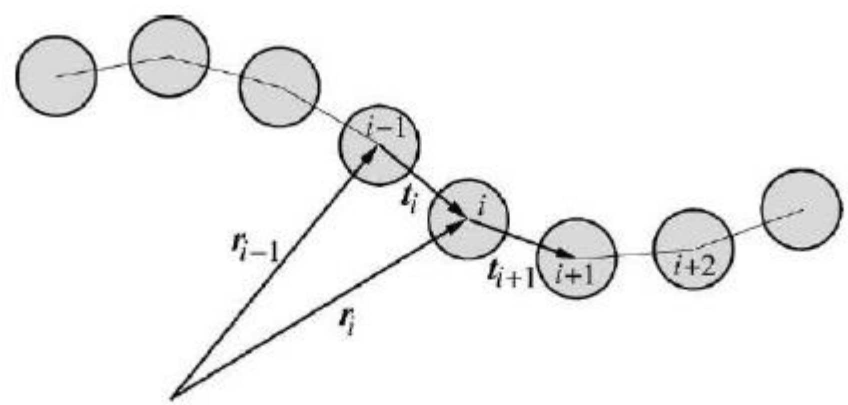
Persistence length: 3,44 μm
Contour length: 34,49 μm
(TIRF micrograph)

Hydrodynamics modeling

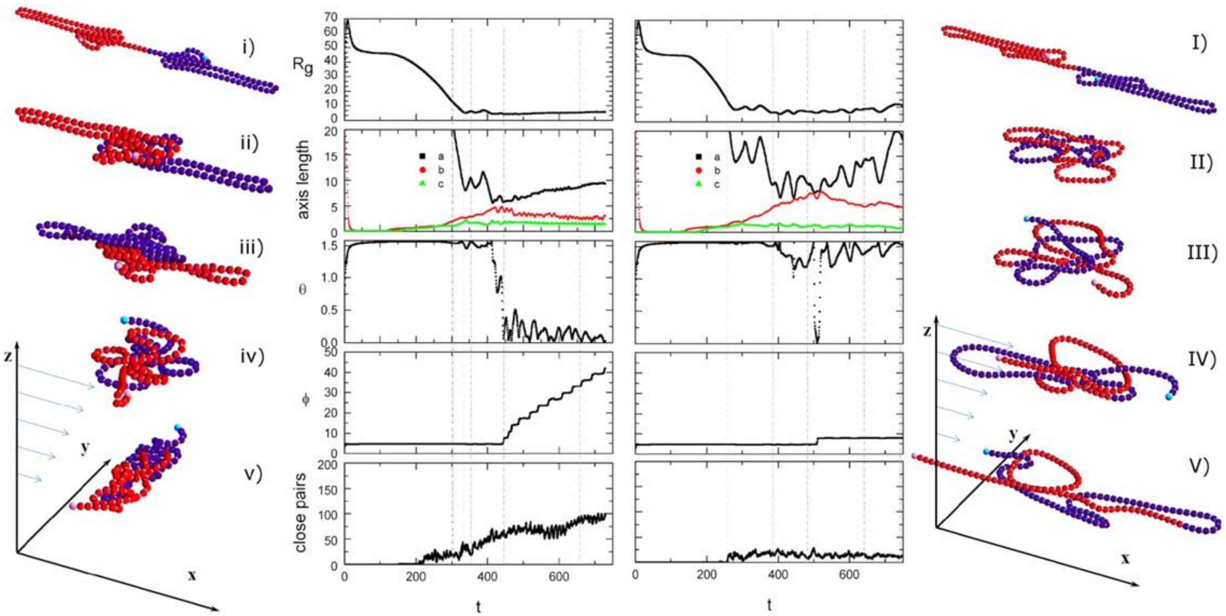
$$\begin{aligned} \eta\nabla^2\mathbf{v} - \nabla p &= \mathbf{0}, \\ \nabla\cdot\mathbf{v} &= 0, \end{aligned}$$

Chain of spheres in Stokes approximation





Hydrodynamics simulations

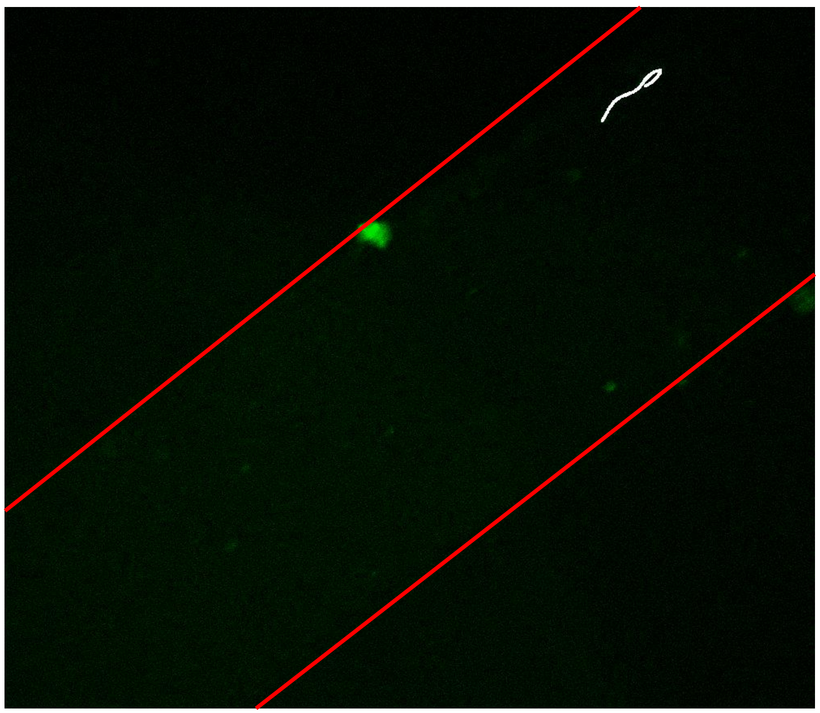


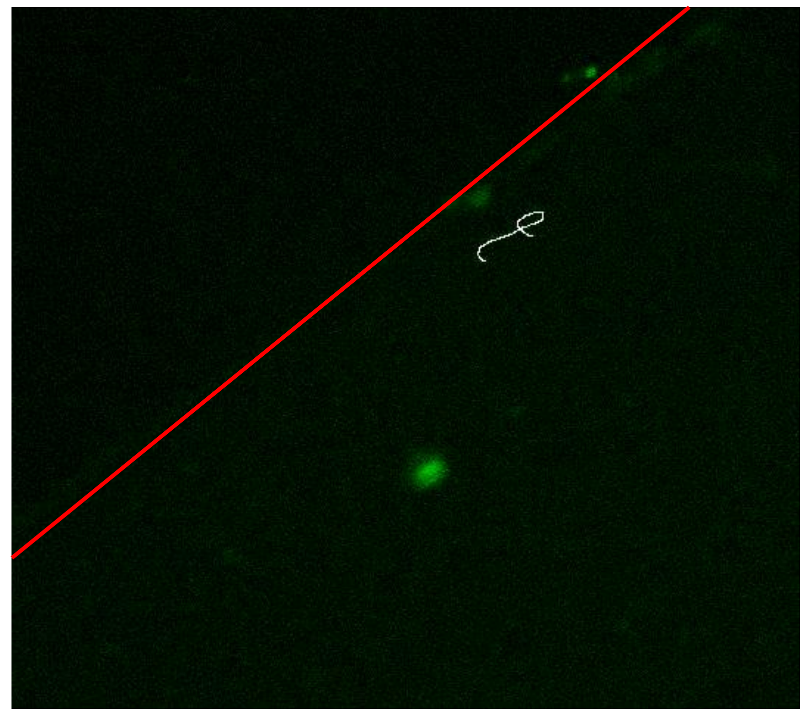
Dynamics and topology of a flexible chain: knots in steady shear flow, Kuei, Slowicka et al. New Journal of Physics 2015;

Is it DNA, or rather, does it simulate the hydrodynamics of a nanofiber?

Hydrogel filaments in flow

Highly flexible PNIPAAm hydrogel nanofilament in flow

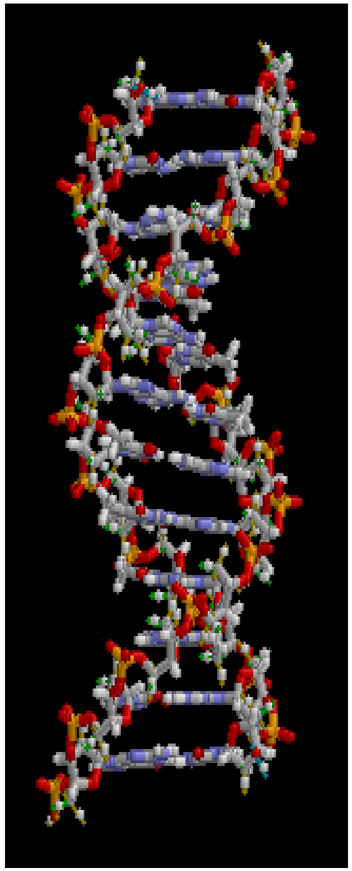




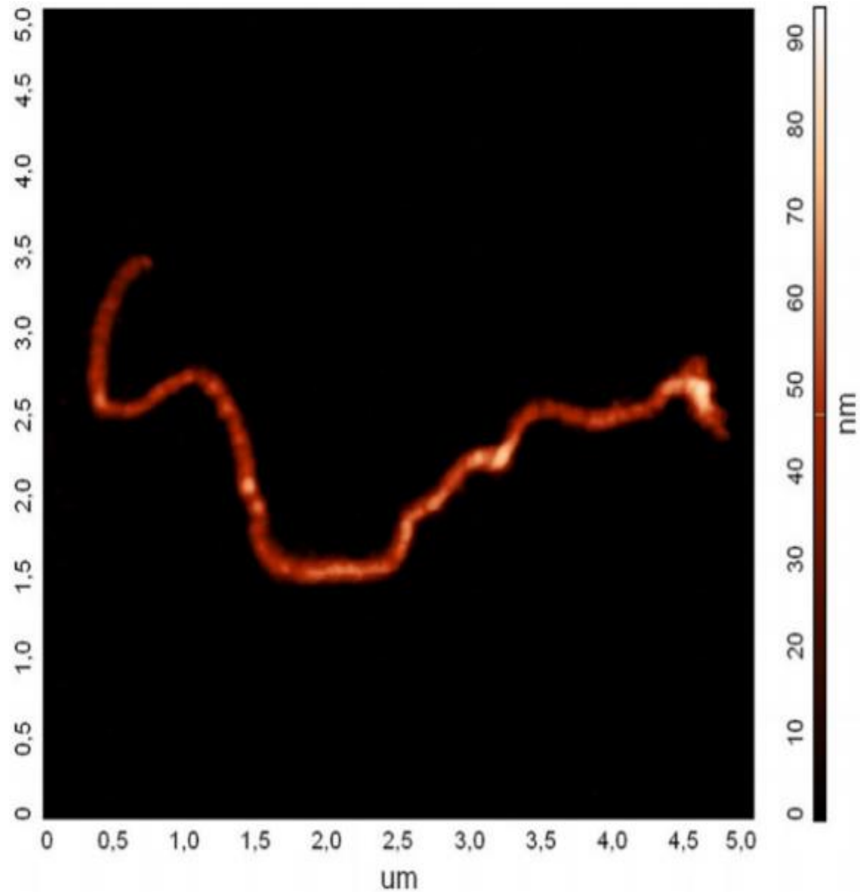
$U = 45\mu m/s$, $L_c = 25\mu m$, $2R = 100nm$, $D = 100\mu m$, $Re_D = 4 \cdot 10^{-3}$

DNA vs. Micro- Nanofibers

2 m!



Edwards KJ, Brown DG, Spink N, Skelly JV, Neidle S.



Pawłowska S., Kowalewski T.A., Pierini F. 2018

DNA: 2×10^{-10} m

Nanofibers: 0.1×10^{-7} m

Conclusions

- DNA in humans (approx. 2 meters) containing about 6.4 billion base pairs is stored tightly packed inside the cell nucleus. The nucleus is enveloped in a membrane separating the nucleoplasm from the rest of the cell.
- The mechanical environment, such as contact with extracellular nanofibers, can influence the physical shape and internal structure of the DNA inside the nucleus.
- **However, engineered nanostructures, both experimental using polymer micro –nanofibers, as well as simple computer models (e.g. a chain of spherical beads), lack of the fundamental properties of DNA are not able to explain the biology of DNA in regulating, storing, and controlling life on our planet.**

FINAL REMARKS

- DNA confined to nanochannels is stretched to near its full contour length. Importantly, this stretching takes place at equilibrium, without any chemical modifications to the DNA extracted from cells.
- The packaging of DNA in cells is important in the realization of all types of biological functions. The compact forms of long DNA, such as supercoils, knots, chromatin and chromosomes, are central to fundamental mechanisms for replication, transcription and recombination.
- **Fluid mechanics may help with its specific tools to characterize, estimate and same time even measure short DNA immersed in liquids.**

Thank you very much for Your attention!

Special thanks to

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Krzysztof Zembrzycki

… and all other colleagues and collaborators from our and other labs!

How *AI* explains reading, copying and repairing DNA