

# Dynamic Simulation of a Polymer Molecule Using Multiphysics: DNA Separation in a Microchannel

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**Introduction:** Entropic trapping DNA separation is used in a wide array of. This is the first trial, where COMSOL Multiphysics® is used to simulate polymer dynamics.

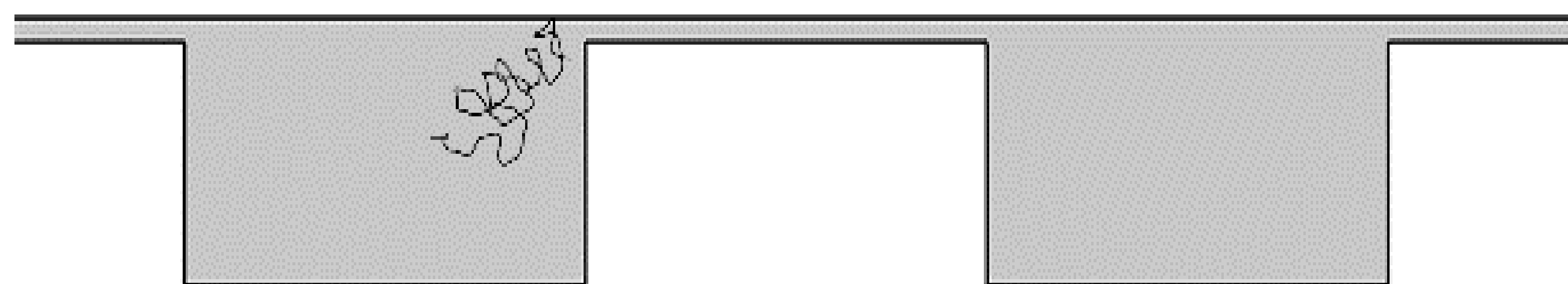


Figure 1. Title of the figure

**Computational Methods:** In this study, a Brownian dynamics (BD) simulation was performed using a coarse-grained bead-spring model to represent the semi-flexible dynamic nature of a  $\lambda$ -DNA molecule in the entropic trap channel.

The bead positions are determined by calculating sum of imposed forces on the beads at each time step.

$$\frac{d}{dt} \left( m_p \frac{dr_i}{dt} \right) = F_i^D + F_i^B + F_i^S + F_i^E + F_i^V$$

Where,  $F_i^D$ ,  $F_i^B$ ,  $F_i^S$ ,  $F_i^E$  and  $F_i^V$  are respectively drag force, Brownian force, spring force, electrical force and excluded volume force.

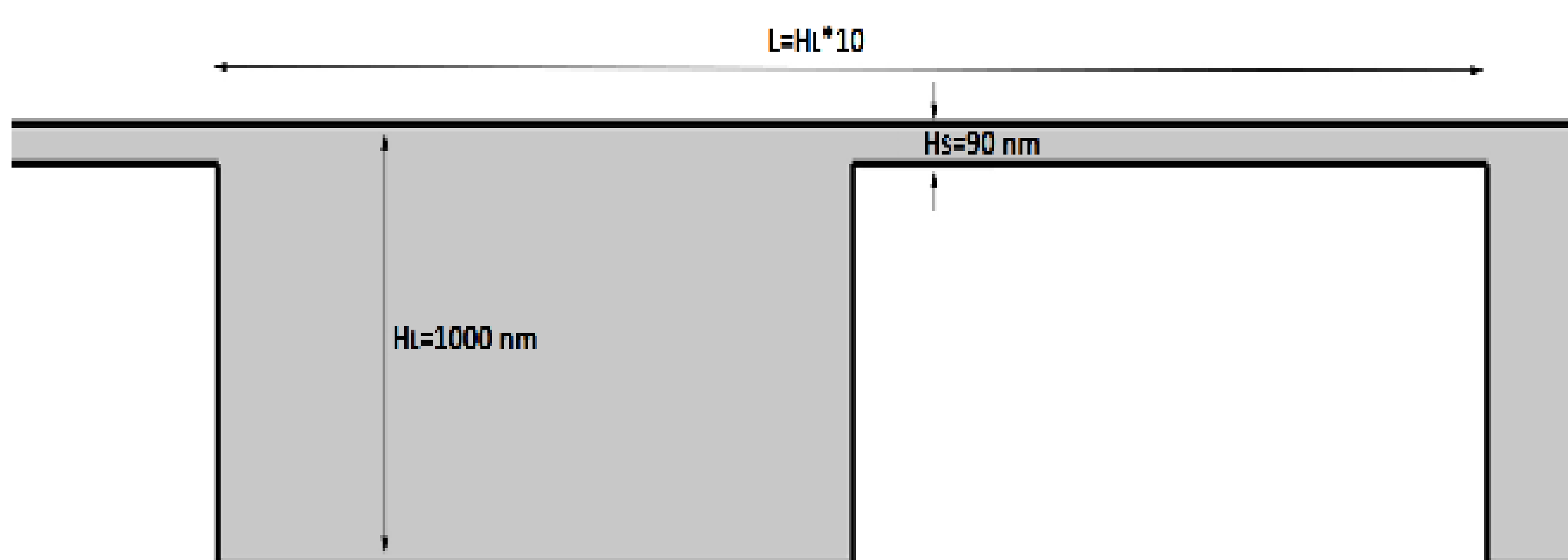


Figure 2. Channel structures used in simulations.

**Results:** The trajectory of DNA chains were simulated in the entropic trap. Our results show qualitative agreement with the experimental observation that the longer DNA elutes faster.

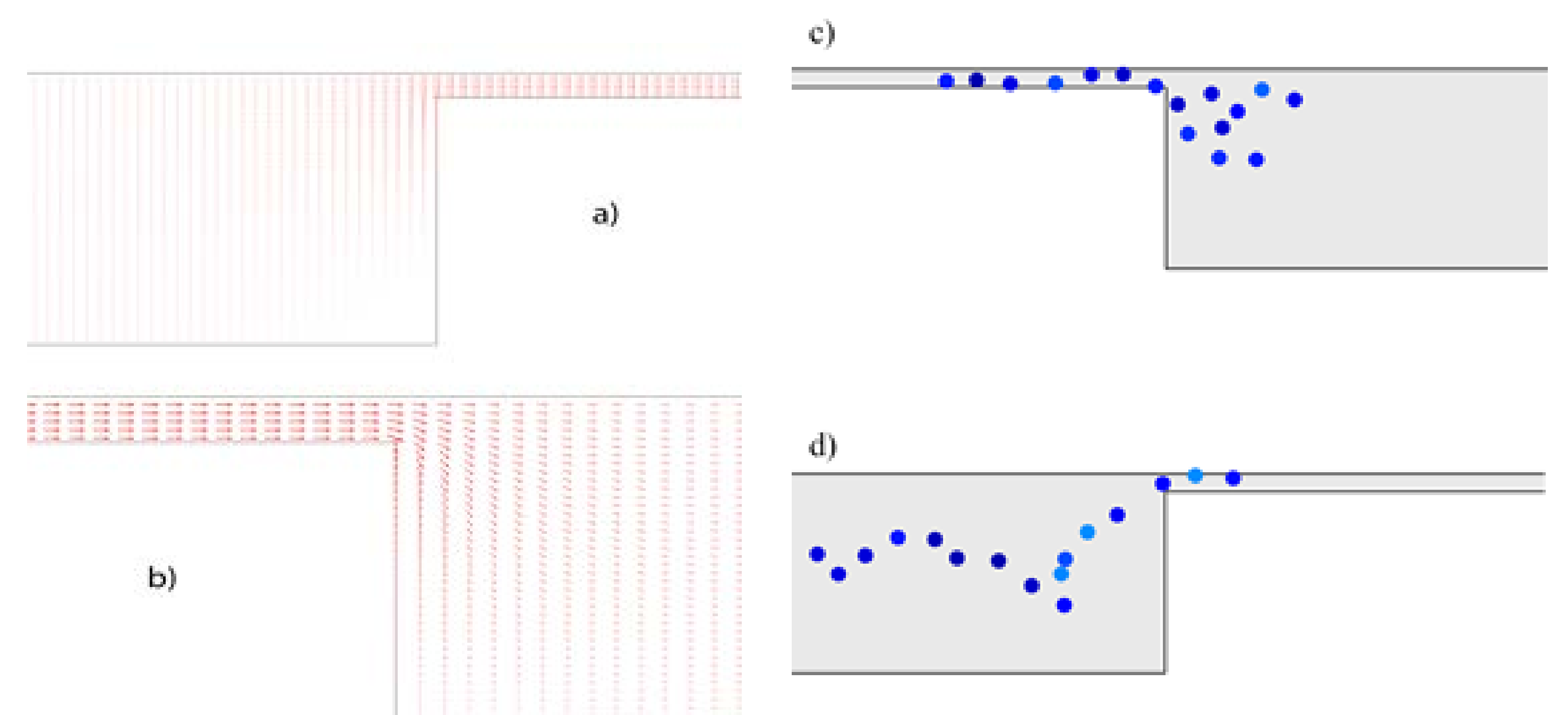


Figure 3. Electrical field flux vectors in (a) the right corner and (b) the left corner of a wide channel. Snapshots of a DNA chain with Nb=16, flowing into (c) and out (d) of a wide channel in an entropic trap

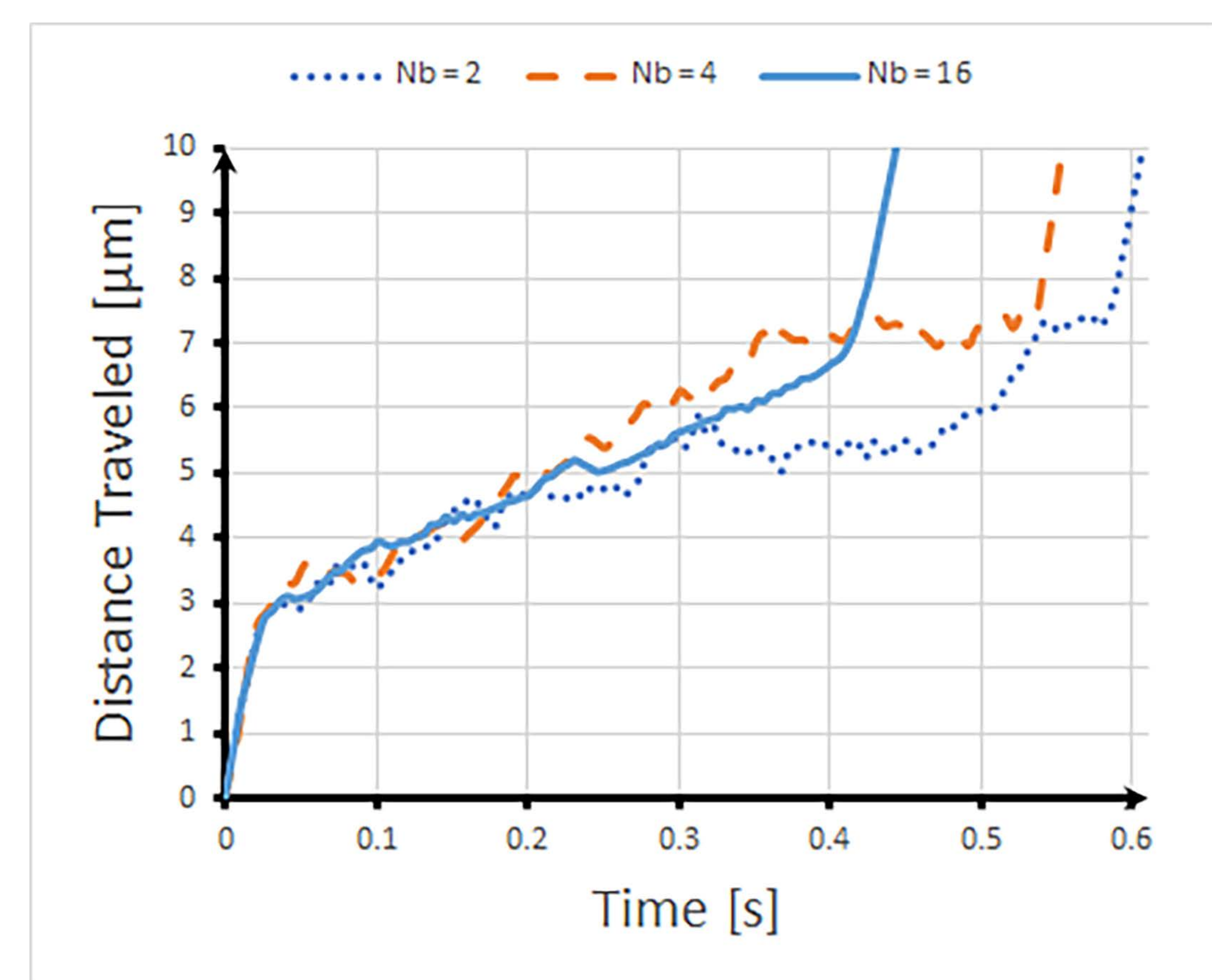


Figure 4. Simulated center-of-mass trajectories of DNA with Nb=2,4 and 16.

**Conclusions:** We performed a Brownian bead-spring simulation of  $\lambda$ -DNAs in a periodically constricted channel. This is the first trial, where COMSOL Multiphysics® is used to simulate polymer dynamics in a micro-fabricated device.

## References:

1. Monjezi, S., Behdani, B., Palaniappan, M.B., Jones, J.D., Park, J., Computational Studies of DNA Separations in Micro-fabricated Devices: Review of General Approaches and Recent Applications, *Advances in Chemical Engineering and Science*, **7**, 362-392 (2017).