Langevin Dynamics Study of Polymer Translocation through a Nanopore

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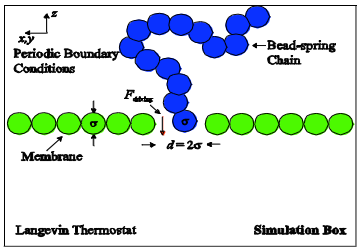
Background

- The study of polymer translocation through a nanopore has attracted attention in recent years, stimulated by the need to understand the ubiquitous biological process of the transport of DNA and RNA between nucleus and cytosol in cells, as well as by the desire to design an efficient DNA sequencing device.
- The physics of the translocation process, however, have not been fully understood. Even on the coarse-grained level (i.e., scaling behavior), theoretical predictions still need to be verified. Computer simulations constitutes a complimentary tool to study the scaling behavior of the polymer translocation process. Specifically, it is our aim to study how the chain length N and the applied driving force F_{driving} affect the scaling behavior of the translocation time τ_{trans} as a function of N. We apply molecular dynamics simulations controlled by a Langevin thermostat.

Simulation Details

Simulations are performed using a modified version of the simulation package LAMMPS.

Illustration of system setup:



- The membrane, composed of one layer of fixed particles of diameter σ, is oriented perpendicular to the z-axis. It contains a pore of diameter 2σ.
- The polymer is modeled by means of the bead–spring model.
- Periodic boundary conditions are applied in all three spatial directions.
- An external driving force F_{driving} is applied to the monomers within pore. Its strength is varied between 0.01 and 3.0 $k_{\text{B}}T/\sigma$.

Monomer–monomer interaction:

$$U_{\text{LJ}} = 4k_{\text{B}}T\left\{\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \frac{1}{4}\right]\right\}, r < \sqrt[6]{2}\sigma$$

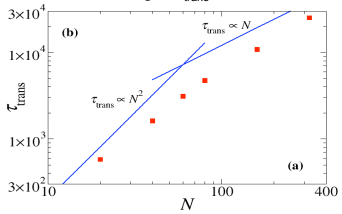
Bond potential:

$$U_{\text{bond}} = 200\frac{k_{\text{B}}T}{\sigma^2}\left(r - \sqrt[6]{2}\sigma\right)^2$$

Results

(Quasi-)Equilibrium system : $F_{\text{driving}} = 0.05\ k_{\text{B}}T/\sigma$

Scaling of τ_{trans} with N



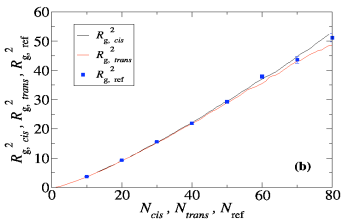
Predictions for equilibrium systems:

$$\tau_{\text{trans}} \propto \begin{cases} N, & N|\Delta\mu| >> k_{\text{B}}T; \\ N^2, & N|\Delta\mu| = 0. \end{cases}$$

$$\Delta\mu \propto F_{\text{driving}}$$

M. Muthukumar, *JCP* **111**, 10371 (1999)

R_g^2 of *cis* and *trans* parts for $N = 80$



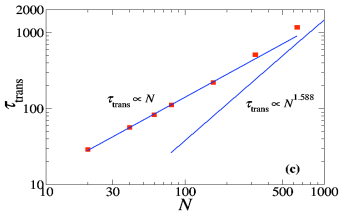
Equilibrium conditions:

$$\tau_{\text{relax}} < \tau_{\text{trans}} / N$$

Lubensky & Nelson, *Biophys. J.* **77**, 1824 (1999)

Non-equilibrium system: $F_{\text{driving}} = 3.0\ k_{\text{B}}T/\sigma$

Scaling of τ_{trans} with N



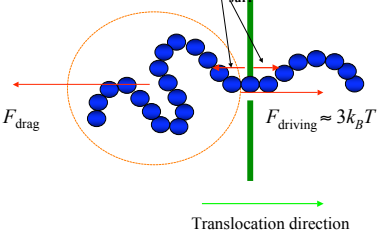
Scaling limit at large N is set by the unhindered motion of the chain:

$$\tau_{\text{trans}} \sim \frac{R}{v} \propto \frac{N^{\upsilon}}{\Delta\mu / N} = \frac{N^{1+\upsilon}}{\Delta\mu} \propto N^{1.588}$$

Kantor & Kardar, *PRE* **69**, 021806 (2004)

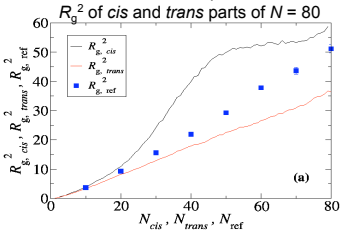
Caveat: Although chain is out of equilibrium, linear scaling is observed here as well!

Surface force $F_{\text{surf}} = -2.4k_BT/\sigma$ (simulation result)

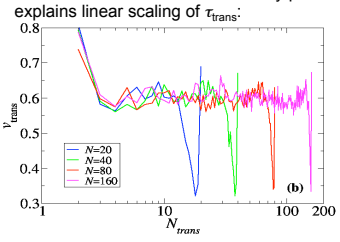


The magnitude of F_{surf} is comparable to F_{driving}, but is ignored in theoretical models. The numbers in this figure apply to the $N = 80$ case.

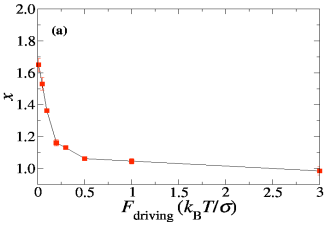
Evidence of out-of-equilibrium chain: R_g^2 of *cis* and *trans* parts of $N = 80$



Instantaneous translocation velocity profile explains linear scaling of τ_{trans}:



Effect of F_{driving} on the scaling exponent x



x is the exponent of the scaling form

$$\tau_{\text{trans}} \propto N^{x}$$

and is measured for $20 \le N \le 80$

Conclusions

- The translocation scaling exponent x ($\tau_{\text{trans}} \propto N^x$) can take values over a wide range, depending on N and F_{driving}.
- At small F_{driving}, the equilibrium theory correctly predicts the scaling behavior, which is dependent on $N|\Delta\mu|$.
- At large F_{driving} (highly non-equilibrium system), a linear scaling is recovered. This might be explained by the presence of a non-negligible surface interaction F_{surf}, which is not considered in any theoretical model. In the large chain length limit, however, the scaling exponent is bounded by the corresponding unhindered motion of the chain, as predicted by Kantor and Kardar.

Acknowledgements

This work is supported by the ACS Petroleum Research Fund under Grant No. 38543-G7 and by the NSF through an ITR grant (DMR-03-25939) via the Materials Computational Center at the University of Illinois at Urbana-Champaign. The authors also thank Intel for a generous equipment donation.