

# Mechanizm translokacji łańcuchów w obiektach biologicznych

stan bieżący badań, wyniki i nadchodzące zagadnienia

Sebastian Żurek

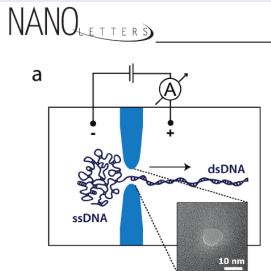
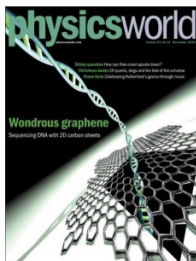
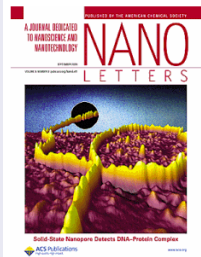
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# Jaki jest mechanizm sterujący transportem protein?



Science 2 December 2005:  
Vol. 310, no. 5753, pp. 1452 - 1456  
DOI: 10.1126/science.1113752

## REVIEW

### Protein Translocation Across Biological Membranes

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Subcellular compartments have unique protein compositions, yet protein synthesis only occurs in the cytosol and in mitochondria and chloroplasts. How do proteins get where they need to go? The first steps are targeting to an organelle and efficient translocation across its limiting membrane. Given that most transport systems are exquisitely

## Translocation of reptating chains

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Received 21 February 2011

Accepted 7 April 2011

Published 4 May 2011

Online at [stacks.iop.org/JSTAT/2011/P05006](http://stacks.iop.org/JSTAT/2011/P05006)  
doi:10.1088/1742-5468/2011/05/P05006

**Abstract.** Voltage-driven translocation is modeled with the Rubinstein-Duke rules for hopping reptons in one- and two-dimensional lattices. The chain is driven through the pore by a bias potential promoting the transition of stored length in one direction. Coupling states give a semi-periodicity of the process that enables us to relate the properties to the stationary state of the master equation. The exact solution for short chains and Monte Carlo simulations for longer chains are used to calculate displacements, velocities and the translocation time.

**Keywords:** classical Monte Carlo simulations, other numerical approaches, polymer dynamics, stochastic processes (theory)

### Acknowledgments

The authors are grateful to G W Barkema for comments and to H W J Blöte for illuminating discussions on the Monte Carlo approach. SŻ thanks the Polish Ministry of Science and Higher Education for supporting this work under the ‘Iuventus Plus’ program (IP2010 050870). Numerical calculations were performed in WCSS Wrocław (Poland, grant 82).

## Translocation of polymers in a lattice model

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January 17, 2012

### Abstract

Voltage-driven polymer translocation is studied by means of a stochastic lattice model. The model incorporates the voltage drop over the membrane as a bias in the hopping rate through the pore and exhibits the two main ingredients of the translocation process: the driven motion through the pore and the diffusive supply of chain length towards the pore on the cis-side and the drift away from the pore on the trans-side. The translocation time is either bias limited or diffusion limited. In the bias-limited regime the translocation time is inverse proportional to the voltage drop over the membrane. In the diffusion-limited regime the translocation time is independent of the applied voltage, but it is rather sensitive to the motion rules of the model. We find that the whole regime is well described by a single curve determined by the initial slope and the saturation value. The dependence of these parameters on the length of the chain, the motion rules and the repton statistics are established. Repulsion of reptons as well as increase of chain length decrease the throughput of the polymer through the pore. As for free polymers, inclusion of a mechanism for hernia creations/annihilations leads to cross-over from reptation to Rouse dynamics. For the Rouse chain that is experimentally the more relevant case the power-law dependence of the translocation time on the chain length is found.

PACS numbers: 87.15.A-, 87.15.H-, 82.35.Lr

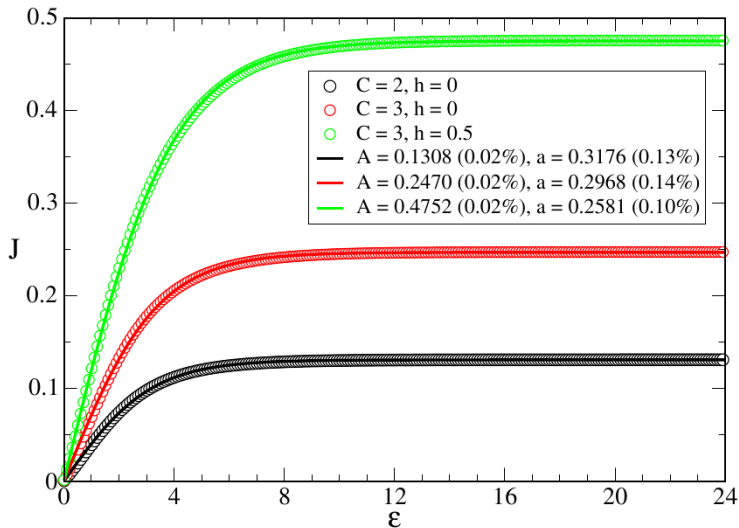
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### 7 Acknowledgements

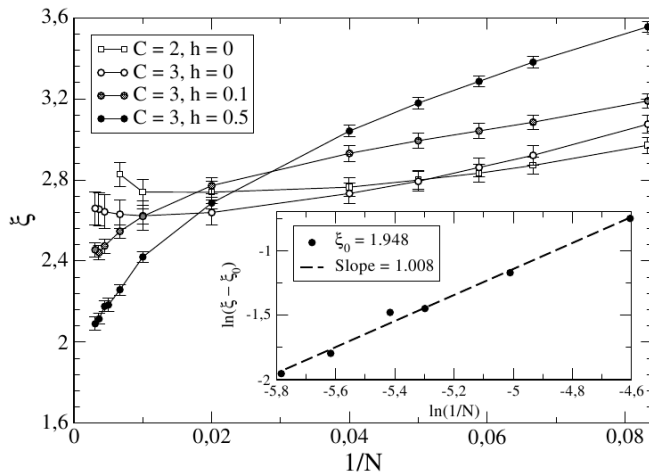
The authors are indebted to discussions with Gerard Barkema, in particular about the asymptotic chain length dependence in the large bias regime. SŻ thanks to the Polish Ministry of Science and Higher Education for supporting this work under the ‘Iuventus Plus’ program (IP2010 050870). Numerical calculations were performed in WCSS Wrocław (Poland, grant 82).



# $J(\epsilon) = A \cdot \tanh(a \cdot \epsilon)$ fit

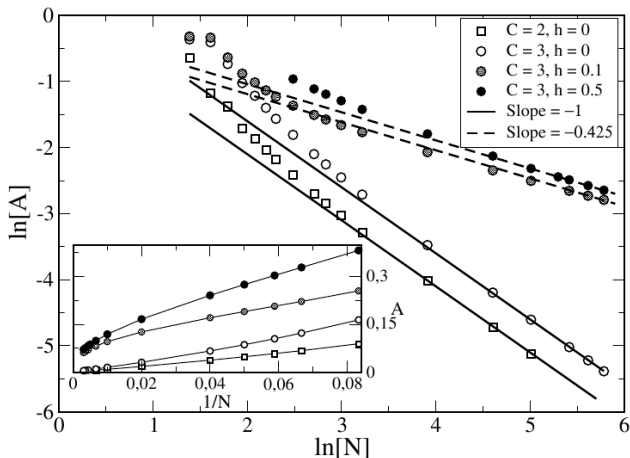


# Obszar ruchu sterowanego (zasilanego)



320 miliardów indywidualnych rekonfiguracji MC

# Transport ograniczany dyfuzją



Jeden punkt: 10 zadań, każde to zazwyczaj 40 procesów MPI

# Czas translokacji dla obszaru ruchu zasilanego

$$A(h) = A_0(h)N^{-(\alpha-1)} + \dots,$$
$$\xi(h) = \xi_0(h) + \xi_1(h)N^{-x} + \dots$$

As argued, the Rouse chain is experimentally the more relevant case. Translated to the translocation time we find for the Rouse chain (using  $\tau = N/J$ ) in the initial regime

$$\tau \sim (c_0 N^{1.43} + c_1 N^{0.43}) \frac{1}{\epsilon}, \quad (9)$$

where we find for  $c_0 = \xi_0/A_0 = 2.4$  and for  $c_1 = \xi_1/A_0 = 49$  at  $h = 0.5$ .

We have included the next term in the expansion, because it has a notable influence for the chain lengths that we consider.

Our previous results [10], obtained by Monte Carlo simulations for shorter chains at  $\epsilon = 2 \ln(2) \sim 1.4$  and  $h = 0.5$  or  $h = 0$ , are in agreement with the present ones.





# Dziękuję!