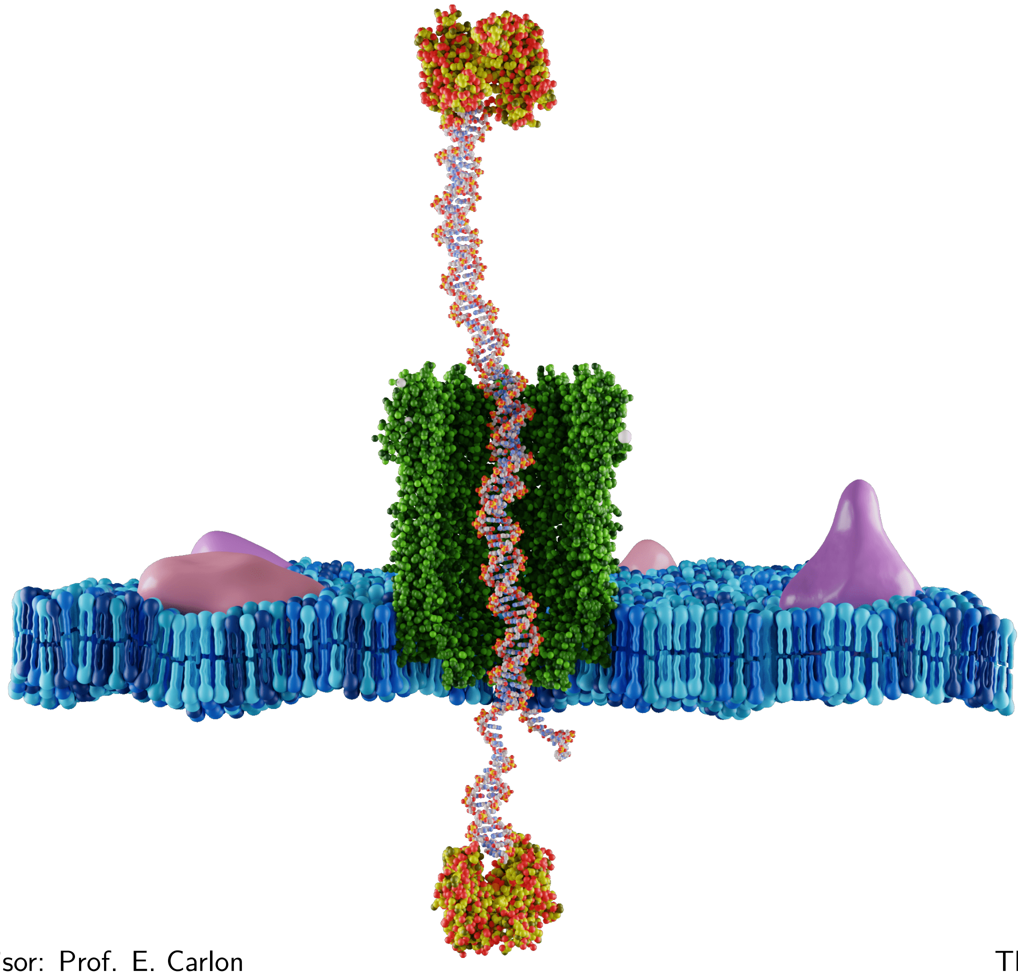
KU LEUVEN

FACULTY OF SCIENCES

Coarse-grained simulations of the DNA nanopiston



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Thesis presented in
fulfillment of the requirements
for the degree of Master of Science
in Physics

Academic year 2020-2021

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Abstract

abstract

Vulgariserende Samenvatting

Summary in dutch.

asdf

Summary in Layman's Terms

Summary in english.

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CHAPTER 1

Introduction

...if we were to name the most powerful assumption of all, which leads one on and on in an attempt to understand life, it is that all things are made of atoms, and that everything that living things do can be understood in terms of the jigglings and wigglings of atoms.

— Richard P. Feynman, *The Feynman Lectures on Physics*[2]

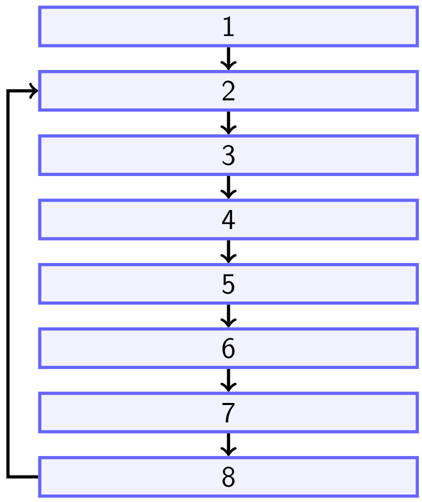
Here why simulation. blik in iets dat we vaak niet zien.

1.1 Deoxyribonucleic Acid

1.2 Polymer Physics

1.3 Computer Simulations

1.3.1 Molecular Dynamics



- understanding many body - newtons algorithm - insight in the dynamics -> simulate trajectories - recent developments in techniques to simulate trajectories of rare event -increased computational power

1.3.2 Coarse Grained modelling

CHAPTER 2

nano pore

asldfkasdflj

CHAPTER 3

Rotaxane

3.1 Mixed Rotaxane

3.1.1 Diffusion approximation

Studying the dynamics of the mixed rotaxane highlighted the importance of entropic interactions between the nano pore and the DNA strand. Here we observed that a fully double stranded DNA polymer represented a special case. The uniformity of the $\mathcal{X}$ histogram corresponding to this 0 nt mixed rotaxane suggests a free diffusive motion of the rotaxane in a bounded one-dimensional domain. This isotropic behaviour was previously also observed in the bead-spring simulations by Bayoumi et al.[1]

$$\langle \Delta x^2 \rangle \simeq 2nDt.$$

$$\frac{\partial \psi}{\partial t} = D\frac{\partial^2 \psi}{\partial x^2}, P(x,t) = f(x)g(t)$$

Reflecting boundary conditions $j = -D\frac{\partial \psi}{\partial x} = 0$. Current vanishes at the boundaries

$$t: \quad \dot{g} = -\alpha g(t) \Rightarrow g(t) = e^{-\alpha t}$$

$$
\begin{aligned}
x: \quad D\ddot{f} = -\alpha f(x) \Rightarrow f(x) &= A\sin(Kx) + B\cos(Kx) \\
&= B\cos(\frac{\pi n x}{L})
\end{aligned}
$$

$$\frac{\alpha}{D} = \frac{\pi^2 n^2}{L^2}$$

The general solution is given by the linear combination,

$$
\begin{aligned}
\psi(x,t) &= \sum_{n=0}^{+\infty} C_n \cos\left(\frac{\pi n x}{L}\right) e^{-\frac{D\pi^2 n^2}{L^2}t} \\
&= \frac{1}{L}\left\{1 + \sum_{n=1}^{+\infty} \cos\left(\frac{\pi n x_0}{L}\right)\cos\left(\frac{\pi n x}{L}\right) e^{-\frac{D\pi^2 n^2}{L^2}t}\right\}
\end{aligned}
$$

$$
\begin{aligned}
\langle \Delta x^2 \rangle &= \langle (x - x_0)^2 \rangle \\
&= \frac{L^2}{6}(1 - \frac{96}{\pi^4}\sum_{n=0}^{+\infty} \frac{1}{(2k+1)^4} e^{-\frac{D(2k+1)^2\pi^2}{L^2}t})
\end{aligned}
$$

As expected, the mean squared distances saturates to $\langle \Delta x^2 \rangle = L^2/6$ in the long-time limit $t \gg L^2/D$.

CHAPTER 4

hybrydisation

asldfkasdflj

CHAPTER 5

Conclusions and Perspectives

5.0.1 asdf

APPENDIX A

First appendix

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[2] Feynman, Richard P. (Richard Phillips), .-. (c1963). The Feynman lectures on physics. Reading, Mass. : Addison-Wesley Pub. Co., c1963-1965. Vol. 2 has subtitle: The electromagnetic field; 3 has subtitle: Quantum mechanics.;Includes bibliographical references and indexes.

Acknowledgements

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