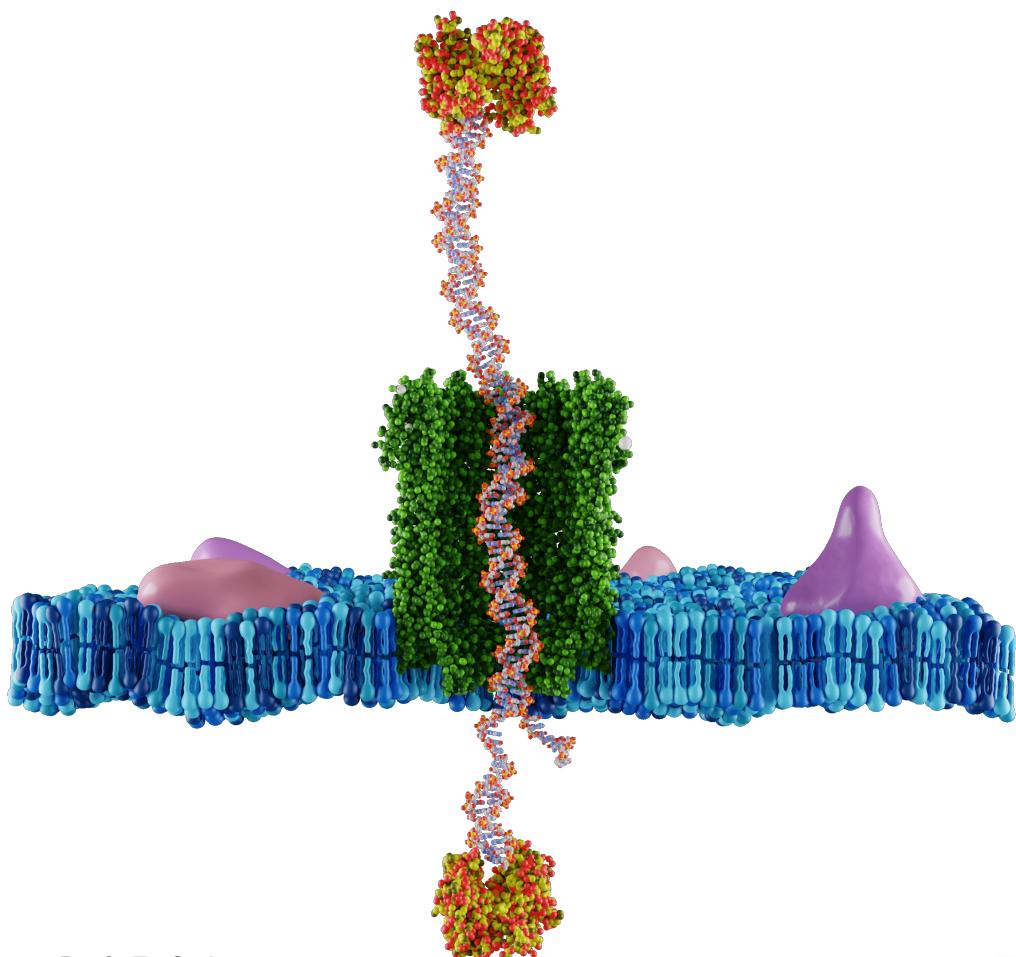


Coarse-grained simulations of the DNA nanopiston

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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

1.1 Deoxyribonucleic Acid

1.2 Polymer Physics

1.3 Computer Simulations

The theory of classical mechanics is often regarded as the first major breakthrough in the field of physics. For every aspiring physicist this is still the starting point of their studies. Unfortunately getting to know these relatively simple laws of nature, leads to the inescapable realisation that these theories are expressed in mathematical formalism that are only analytically solvable in few idealised scenarios. Applying these formulas to a problem consisting of just more than two particles already leads practically unsolvable equations.

Although it is often times not possible to find an exact solution to equations related to complex physical systems, finding reasonable approximations to their solution is. One popular method to analyse the dynamics of complex systems is the use of simulations.

Simulations have a rich history within physics and engineering, starting even before the invention of the computer. An example of one of these mechanical simulations is the Waterloopkundig Laboratorium or currently the waterloopbos, a scale model of important Dutch waterways where the influence of waves on harbours and docks was studied. This simulation played an important part in the design of the famous Delta Works.

Another example is the use of mechanical simulations to study the structure of water. In the early 20th century physicist J.D. Bernal and his fellow researchers build various ball and stick models of water to analyse the possible 3D configurations of water molecules in a liquid. Their research eventually explained the peculiar physical properties of water from a atomistic perspective. However useful these mechanical simulations turned out to be, the biggest drawback of the method was the extreme cost of labour to construct them as pointed out by Bernal in his 1962 lecture,

... I took a number of rubber balls and stuck them together with rods of a selection of different lengths ranging from 2.75 to 4 inch. I tried to do this in the first place as casually as possible, working in my own office being interrupted every five minutes or so and not remembering what I had done before the interruption. However, ...



Figure 1.1: Example of an expanded model of a simple liquid (J L Finney, Ph.D thesis)

After the first computer simulations were performed in the Los Alamos labs, the popularity of simulations rapidly increased. The remarkable explanatory power of simulations combined with the relative easy construction of computer models lead to a fast adoption of computer simulations in the scientific community. Within the context of this thesis, computer simulations are used to study the mechanics of the DNA Polymer. Due to the high number of atoms in a typical system, it is generally not possible to find an analytical solution to their equations of motion. In this context, simulations are often used to gain an insight into the complex dynamics of the system and guide the developments of simple approximate theories. The simulations act as a bridge between the microscopic constituents of the systems and the macroscopic properties we want to understand.

1.3.1 Molecular Dynamics Simulations

Molecular Dynamics (MD) is a computer simulation technique, used to analyse the dynamics of a classical many-body system. The central idea of this method is to generate all the particle trajectories in a system of N particles by numerically integrating the classical equations of motion,

$$m_i \ddot{\mathbf{r}}_i = \mathbf{f}_i, \quad \mathbf{f}_i = -\frac{\partial}{\partial \mathbf{r}_i} \mathcal{U}, \quad \text{for } i \in N.$$

Solving these differential equations is then achieved by employing a discretized time integration scheme. Algorithm 1 shows the typical structure of a molecular dynamics simulations. The discretization resolution is conventionally called the time step of the simulations denoted by Δt . The integration scheme we use depends on the system we want simulate. For isolated systems an energy conserving integration scheme is needed, a popular example is the velocity-Verlet algorithm is. If on the other hand a

- thermostats
- Integrations schemes
- Rare event sampling
- 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

Algorithm 1: The Velocity Verlet algorithm

```

Input : Configuration of the system at  $t = 0$ 
Output : Configuration of the system at  $t = t_f$ 
1 newList = [ ]
2 /* For odd elements in the list, we add 1, and for even
   elements, we add 2. After the loop, all elements are even.
   */
3 for  $i \leftarrow 0$  to  $n - 1$  do
4   if isOddNumber( $a_i$ ) then
5     | newList.append( $a_i + 1$ )           // Some thought-provoking comment.
6   else
7     | // Another comment
8     | newList.append( $a_i + 2$ )
9   end if
10 end for
11 return newList
```

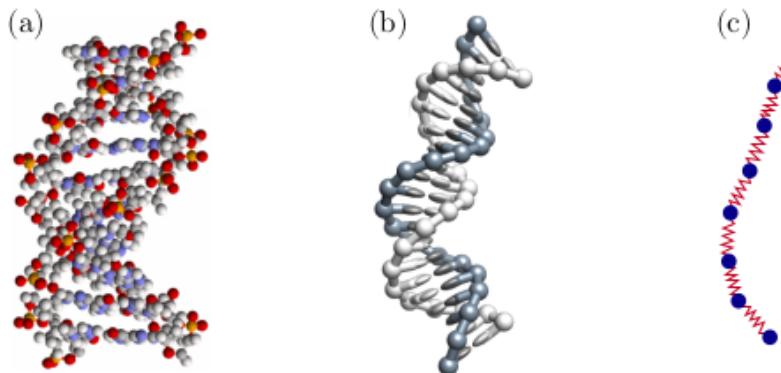


Figure 1.2: zelf nog namaken met blender!!!

CHAPTER 2

nano pore

asldfkasdflj

CHAPTER 3

Methods

Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective positions of the beings which compose it, if moreover this intelligence were vast enough to submit these data to analysis, it would embrace in the same formula both the movements of the largest bodies in the universe and those of the lightest atom; to it nothing would be uncertain, and the future as the past would be present to its eyes.

— Pierre-Simon Laplace

3.1 Figures

An example is Figure 3.1

3. METHODS

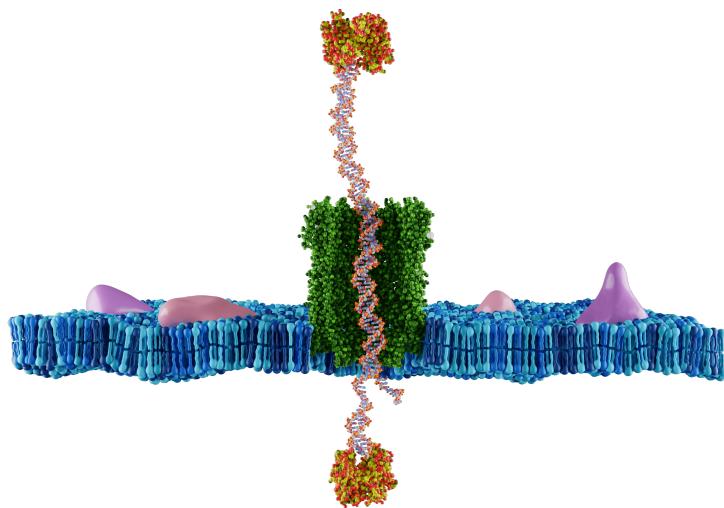


Figure 3.1: A landslide.

3.2 Tables

An example is Table 3.1

Model	Accuracy
regression	90%
random forests	95%

Table 3.1: A random table.

3.3 Equations

Equations can be inserted in the text itself, working in the *mathmode*(put text between \$-signs, for example $Y_i = \frac{1}{x}$). Or put them in the text as a numbered floating element (e.g. Equation (3.1)).

$$y = \frac{1}{x} \quad (3.1)$$

$$y = \int_a^b x^2 dx \quad (3.2)$$

$$y = \sum_{i=1}^n x_i^2 \quad (3.3)$$

You can align the equations:

$$y = \frac{1}{x} \quad (3.4)$$

$$y = \int_a^b x^2 dx \quad (3.5)$$

$$y = \sum_{i=1}^n x_i^2 \quad (3.6)$$

CHAPTER 4

Rotaxane

4.1 Mixed Rotaxane

4.1.1 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

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

$$x : D\ddot{f} = -\alpha f(x) \Rightarrow f(x) = A \sin(Kx) + B \cos(Kx) \\ = B \cos\left(\frac{\pi n x}{L}\right)$$

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

The general solution is given by the linear combination,

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

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

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 5

hybrydisation

asldfkasdflj

6

CHAPTER

Conclusions and Perspectives

6.0.1 asdf

APPENDIX

A

First appendix

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Autonomous and active transport operated by an entropic dna piston. Nano Letters, 21(1):762–768. PMID: 33342212.

- [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.

- [1] Bayoumi, M., Nomidis, S. K., Willems, K., Carlon, E., and Maglia, G. (2021).

Bibliography

Acknowledgements

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