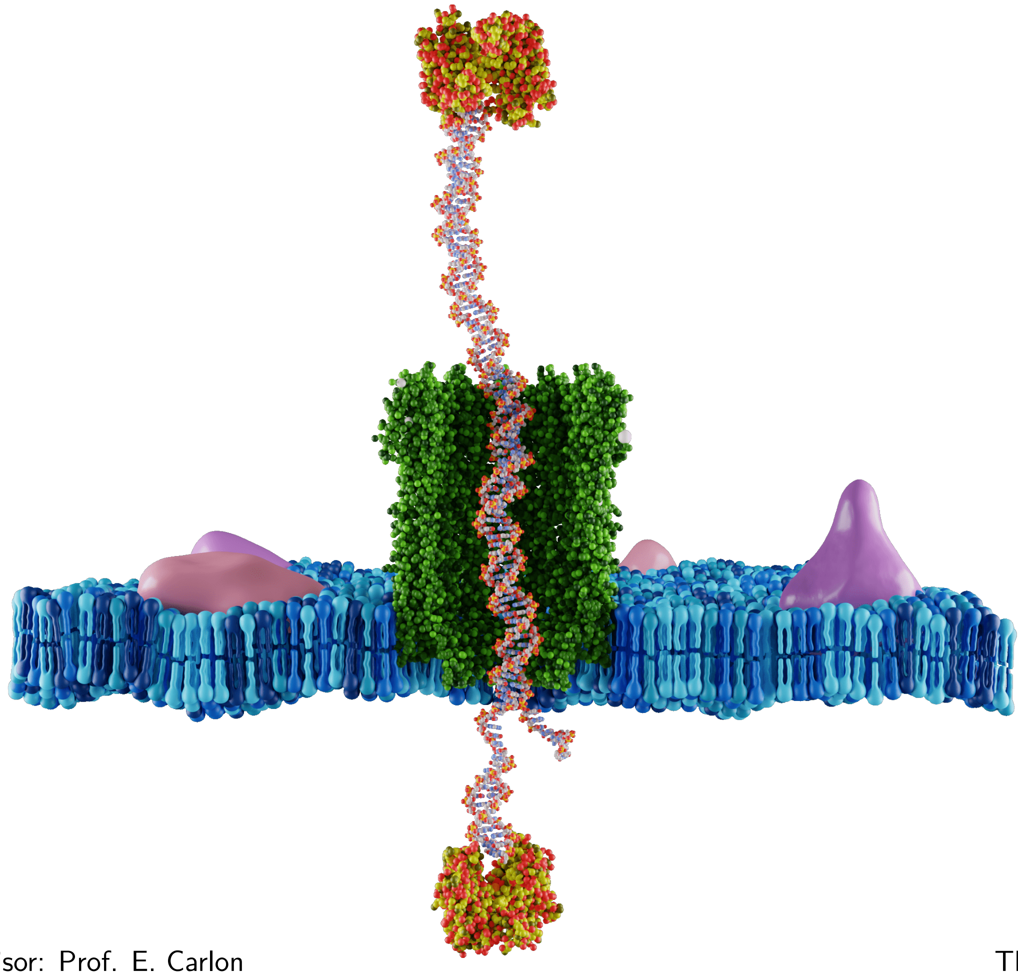
KU LEUVEN

FACULTY OF SCIENCES

Coarse-grained simulations of the DNA nanopiston



Jan Stevens

Supervisor: Prof. E. Carlon
Affiliation *(optional)*

Tutor: *(optional)*
Affiliation *(optional)*

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

Academic year 2020-2021

Abstract

abstract

Vulgariserende Samenvatting

Summary in dutch.

asdf

Summary in Layman's Terms

Summary in english.

List of Figures

List of Tables

Contents

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 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. Already when trying to apply these formulas to a problem consisting of just more then two bodies the equations become practically unsolvable, this fact has vexed physicists and mathematician for many years.

Although it is often times not possible to find an exact solution to many equations encountered in physics, finding reasonable approximations to their solution is. Various types of techniques are used to find these approximations, ranging from taylor expansions to simulations. Before the invention of computers these simulations where performed mechanical and consisted of large amounts of

> . . . 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,. . .

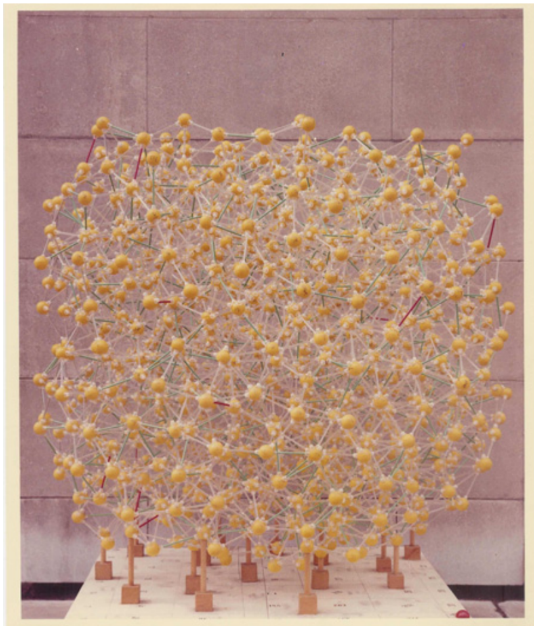


Figure 1.1: Example of an expanded model of a simple liquid (J L Finney, Ph.D thesis)

mechanical simulations -> bernal

computer simulations -> los alamos, fast adaptation by industry.

Biophysics / consedmatter physics, many body systems, bridge between the micro scopic and macro scopic

1.3.1 Molecular Dynamics Simulations

Molecular Dynamics Simulations (MD) is a computer simulation techniques used to analyse the dynamics of a classical many-body system. In a system with N particles the motion

The central idea is that the trajectories of a system of N particles can be generated over time by numerically integrating the classical equations of motion.

- Iterating Newton laws of physics

$$m_i \ddot{\boldsymbol{r}}_i = \boldsymbol{f}_i, \quad \boldsymbol{f}_i = -\frac{\partial}{\partial \boldsymbol{r}_i} \mathcal{U}$$

- thermostats

- Integrations schemes

- Rare event sampling

Algorithm 1: The Velocity Verlet algorithm

```
Input  : Configuration of the system at t = 0
Output : Configuration of the system at t = t_f
newList = [ ]
/* For odd elements in the list, we add 1, and for even
   elements, we add 2.  After the loop, all elements are even.
   */
for i ← 0 to n − 1 do
    if isOddNumber(a_i) then
        newList.append(a_i + 1)        // Some thought-provoking comment.
    else
        // Another comment
        newList.append(a_i + 2)
    end if
end for
return newList
```

- 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

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

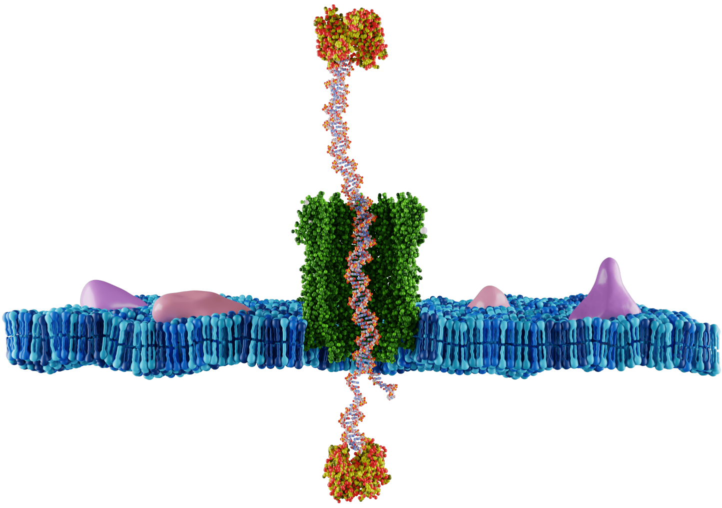


Figure 3.1: A landslide.

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)).

$$y = \frac{1}{x} \tag{3.1}$$

$$y = \int_a^b x^2 dx \tag{3.2}$$

$$y = \sum_{i=1}^{n} x_i^2 \tag{3.3}$$

You can align the equations:

$$y = \frac{1}{x} \tag{3.4}$$

$$y = \int_a^b x^2 dx \tag{3.5}$$

$$y = \sum_{i=1}^{n} x_i^2 \tag{3.6}$$

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

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

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

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

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 5

hybrydisation

asldfkasdflj

CHAPTER 6

Conclusions and Perspectives

6.0.1 asdf

APPENDIX A

First appendix

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetuer.

Suspendisse vel felis. Ut lorem lorem, interdum eu, tincidunt sit amet, laoreet vitae, arcu. Aenean faucibus pede eu ante. Praesent enim elit, rutrum at, molestie non, nonummy vel, nisl. Ut lectus eros, malesuada sit amet, fermentum eu, sodales cursus, magna. Donec eu purus. Quisque vehicula, urna sed ultricies auctor, pede lorem egestas dui, et convallis elit erat sed nulla. Donec luctus. Curabitur et nunc. Aliquam dolor odio, commodo pretium, ultricies non, pharetra in, velit. Integer arcu est, nonummy in, fermentum faucibus, egestas vel, odio.

Bibliography

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

Acknowledgements

...

DEPARTEMENT NATUURKUNDE EN STERRENKUNDE
Celestijnenlaan 200d bus 2412
3000 LEUVEN, BELGIË
tel. + 32 16 32 71 24
fys.kuleuven.be