

SIMULATION OF DIFFUSION IN HETEROGENEOUS MEDIA

by

Paul Ionele

A dissertation submitted to the University of Ontario
Institute of Technology in accordance with the
requirements of the degree of Bachelor of Science
(Hons) in the Faculty of Science.

March 20, 2016



Copyright © 2016 Paul Ionele

ABSTRACT

This is a short example of an abstract.

ACKNOWLEDGEMENTS

Thank some people that you like here.

AUTHOR'S DECLARATION

I declare that the work in this thesis was carried out in accordance with the regulations of the University of Ontario Institute of Technology. The work is original except where indicated by special reference in the text and no part of the dissertation has been submitted for any other degree. Any views expressed in the dissertation are those of the author and in no way represent those of the University of Ontario Institute of Technology. The thesis has not been presented to any other University for examination either in Canada or elsewhere.

Paul Ionele
March 20, 2016

Contents

Abstract	ii
Acknowledgements	iii
Author's Declaration	iv
Table of Contents	v
List of Figures	vi
List of Tables	vii
1 Introduction	1
1.1 Diffusion	1
1.2 Monte Carlo Simulations	1
1.3 Finite Difference (Master Equation) Simulations	1
1.4 Simple Cell Model	2
1.5 A sample introduction	3
1.5.1 A subsection example	3
2 Simulations	5
2.1 1-Dimensional Systems	5
2.1.1 Homogenous System	5
2.1.2 Heterogeneous System	5
2.2 2-Dimensional System	5
3 Results and Analysis	6
4 Future Work and Conclusion	7
References	8
A Appendix	9

List of Figures

1.1	Composite cell showing various important and common internal cell structures. The cytosol fluid occupies the largest portion of volume within the cell.	2
1.2	Density profiles of various models	4

List of Tables

1. INTRODUCTION

What was/is the purpose of this thesis? Why did we develop these computational simulations? Really, we need a goal!

In this thesis, a lattice Monte Carlo approach was used to simulate diffusion. Also used a finite difference method to simulate diffusion. Both problems were boundary-value problems.

We also performed an analysis: MSD, mean position, etc.?? Analysis is kind of empty!

Overall overview to thesis? What kind of an overview? Or just a general background to some main concepts needed or used in this thesis? How does this compare with the abstract?

1.1 Diffusion

Say something general

1.2 Monte Carlo Simulations

1.3 Finite Difference (Master Equation) Simulations

This was done in 1D and 2D.

1.4 Simple Cell Model

Nearly all human cells are microscopic in size; their diameters range from $7.5\text{ }\mu\text{m}$ to approximately $150\text{ }\mu\text{m}$ and a cell exhibits a particular size or shape that reflects the specific task it's designated to perform. There are many different types of cells including nerve cells, muscle cells, and gland cells, but despite their anatomical and functional differences, the cells of the human body have many similarities. It is a fact that no cell contains all cellular components found in all the cell types, so often a *composite cell* is used to exhibit the most important characteristics. Each cell is enclosed by a plasma membrane that separates the cell from the surrounding environment. The inside of the cell is largely composed of a gel-like substance that is dense arrangement of proteins, organelles, and other molecules, suspended in a watery fluid called cytosol. The dense crowding of molecules and organelles results in frequent physical interactions, therefore promoting metabolic efficiency (Patton, Thibodeau , 2013).

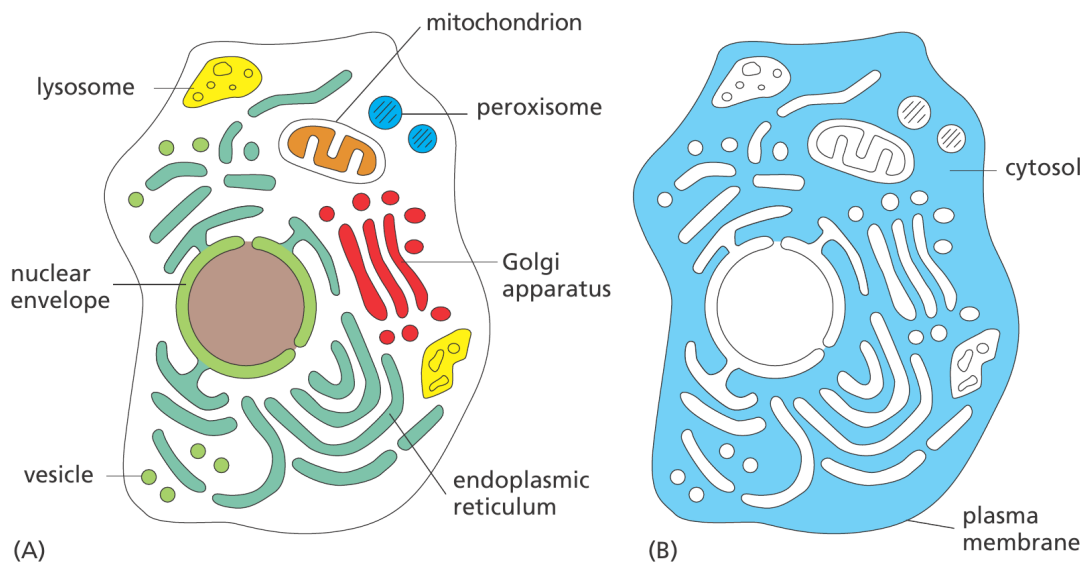


Figure 1.1: Composite cell showing various important and common internal cell structures. The cytosol fluid occupies the largest portion of volume within the cell.

In a multicellular organism, there are several levels of biological organization. A

cell is the lowest level of organization that is considered living; tissues are the next higher level of organization and are composed of cells similar in structure and function. This ensemble of cells resides in an extracellular matrix (ECM); a medium containing water, fibrous and adhesive proteins, glycoproteins, and other molecules. The ECM varies in composition between different tissues, but providing structural support and facilitating cell-to-cell communication are common functions of the ECM. Normally, the cytoplasm is more viscous than the extracellular matrix. (Campbell, Reece , 2008).

1.5 A sample introduction

This is just an example, but I wanted to show you some common things to do with Latex.

1.5.1 A subsection example

For of all, here's an equation – it's the NFW formula, given by Navarro, Frenk, & White (1995), and looks like

$$\rho(r) = \frac{\rho_s}{r/r_s(1 + r/r_s)^2}, \quad (1.1)$$

where ρ_s and r_s are a characteristic density and scale radius, respectively.

Now, I can reference that equation later, since it's labelled properly; it's equation (1.1). Notice that I cited a paper above; I could do that in a different way like this (Navarro, Frenk, & White, 1995).

Just one other quick thing: figures. There's one below, and again it's properly labelled. It's Figure 1.2.

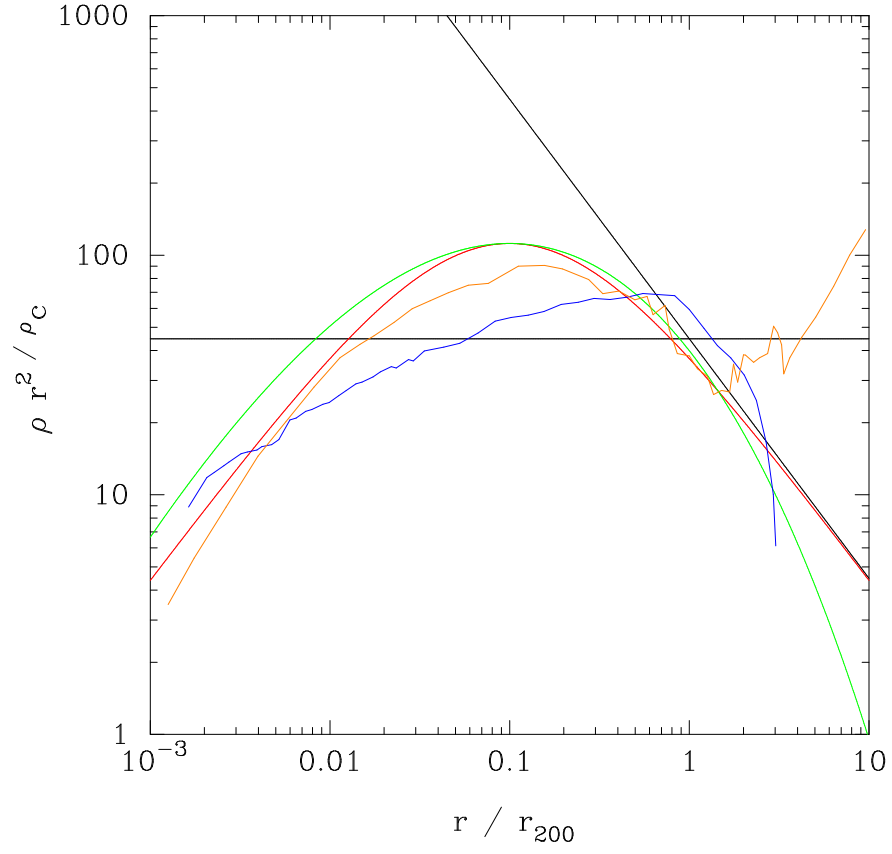


Figure 1.2: Density profiles, shown as ρr^2 to better highlight the differences, of various models.

2. SIMULATIONS

A simulation is intended to imitate—in many cases—a real-world process or system. Before any such simulation can begin, a model of the system studied must be constructed. In general, a model should be as simple as possible while still explaining experimental observations and make predictions with a given degree of accuracy. Models contain key characteristics and behaviours of the system they represent and the simulation is the implementation of the model intended for testing, analysis, and/or visual presentation.

2.1 1-Dimensional Systems

In 1D, homogenous and heterogeneous simple cell systems were simulated using Monte Carlo (MC) and finite difference approaches.

2.1.1 Homogenous System

include figure of homogenous model

2.1.2 Heterogeneous System

include figure of heterogeneous model

2.2 2-Dimensional System

include figure of heterogeneous model

3. RESULTS AND ANALYSIS

4. FUTURE WORK AND CONCLUSION

May just put this into the results section near the end as conclusions and future work.

REFERENCES

Navarro, J.F., Frenk, C.S., & White, S.D.M. 1995, MNRAS, 275, 720

Campbell, N.A., Reece, J.B., et al. 2008. Biology. 8th ed. Pearson Benjamin Cummings.

Patton K.T., Thibodeau G.A.. 2013, 8th ed. Elsevier.

A. APPENDIX

This is just an example of an appendix.