

LATEX Template for Thesis

A dissertation submitted to the Graduate School
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Doctorate of Philosophy

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by

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Abstract

ABSTRACT

To all suffering PhD students.

Acknowledgment

ACKNOWLEDGMENT

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List of Abbreviations

CHARMM Chemistry at Harvard Macromolecular Mechanics

LAMMPS Large-scale Atomic/Molecular Massively Parallel Simulator

NAMD Nanoscale Molecular Dynamics

Chapter 1

Introduction

1.1 Molecular dynamics packages

CHARMM[1], LAMMPS[3] and NAMD[2].

1.2 Organization of thesis



Figure 1.1: Image credit: <https://www.latex-project.org/>

Chapter 2

Logo of CHARMM

2.1 Methods



Figure 2.1: Image credit: <https://embnet.vital-it.ch>

2.2 Conclusions

Chapter 3

Logo of LAMMPS

3.1 Methods

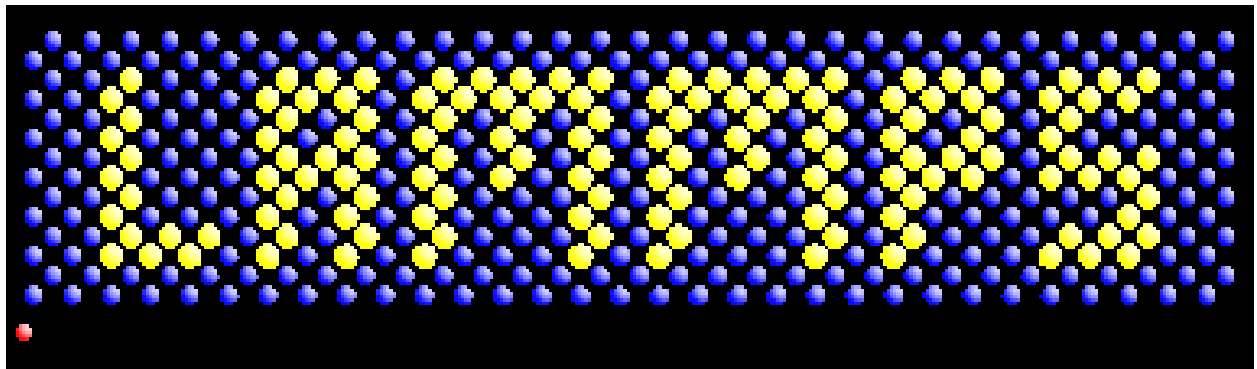


Figure 3.1: Image credit: <https://lammps.sandia.gov/>

3.2 Conclusions

Chapter 4

Logo of NAMD

4.1 Methods



Figure 4.1: Image credit: <https://www.ks.uiuc.edu/Research/namd/>

4.2 Conclusions

Chapter 5

Conclusions

Table 5.1: Chapters of molecular dynamics package names

Chapter	name
2	CHARMM
3	LAMMPS
4	NAMD

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