Parallelization of classical molecular dynamics with OpenMP

Samuel Moerman

Dept. of Computer Science

New York University

New York, USA

shm9853@nyu.edu

Anway Agte
Dept. of Computer Science
New York University
New York, USA
ama10345@nyu.edu

Atmaj Koppikar

Dept. of Computer Science

New York University

New York, USA

ark9238@nyu.edu

Mihir Prajapati

Dept. of Computer Science

New York University

New York, USA

jo1449@nyu.edu

Abstract—We will parallelize a molecular dynamics simulation

Index Terms—OpenMP, Molecular Dynamics

I. INTRODUCTION

I LOVE OPENMM. [1]

REFERENCES

[1] Peter Eastman and Vijay Pande. Openmm: A hardware-independent framework for molecular simulations. *Computing in science & engineering*, 12(4):34–39, 2010.