

# CHE665 Report

Prateek Kumar Pandey(200710) and Anshul Mehta(200154)

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## 1 Introduction

In this project, we have used a commercial molecular dynamics package (lammmps) to perform NPT simulations of a  $15 \times 15 \times 15$  box filled with water molecules at 300 K and 1 atm. We have used SPC or TIP4P, or TIP5P water model for our system to compute the radial distribution function of water and compare it to experimental results