Molecular Dynamics with C++ report

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1 Introduction

Molecular dynamics simulations are becoming an essential part of modern technology, because they allow to study the behavior of complex systems in a controlled way. The simulation of molecular systems is a very complex task, because the number of atoms in a system can be very large. Therefore, the simulation of a system requires a lot of computational power. In the last years, the computational power of computers has increased dramatically. This development has led to the fact that molecular dynamics simulations are now possible for systems with millions of atoms. However, the simulation of such systems is still a very demanding task. Therefore, the simulation of such systems is usually done on supercomputers or clusters of computers.

In this report, we will discuss the design and Implementation of a molecular dynamics simulations for atoms and molecules. We will also discuss the different potential forces that are used in the simulations, and how they are implemented, initializing atomic systems in random positions and preserve the atoms from evaporating using Thermostates, how to make the simulation run faster by using only neighbor list search, and how to parallelize the simulation using MPI.

2 Methods

Give a brief overview of the work relevant for your report.

3 Implementation

Explain the math and introduce notation. sds

Figure 1: Use tikz to draw nice graphs!

Algorithm 1 Stochastic Gradient Descent: Neural Network

Create a mini batch of m samples $\mathbf{x}_0 \dots \mathbf{x}_{m-1}$
foreach sample $\mathbf{x}$ **do**
  $\mathbf{a}^{\mathbf{x},0} \leftarrow \mathbf{x}$ ▷ Set input activation
  foreach Layer $l \in \{1 \dots L-1\}$ **do** ▷ Forward pass
    $\mathbf{z}^{\mathbf{x},l} \leftarrow \mathbf{W}^l \mathbf{a}^{\mathbf{x},l-1} + \mathbf{b}^l$
    $\mathbf{a}^{\mathbf{x},l} \leftarrow \varphi(\mathbf{z}^{\mathbf{x},l})$
  end for
  $\boldsymbol{\delta}^{\mathbf{x},L} \leftarrow \nabla_{\mathbf{a}} C_{\mathbf{x}} \odot \varphi'(\mathbf{z}^{\mathbf{x},L})$ ▷ Compute error
  foreach Layer $l \in L-1, L-2 \dots 2$ **do** ▷ Backpropagate error
    $\boldsymbol{\delta}^{\mathbf{x},l} \leftarrow ((\mathbf{W}^{l+1})^T \boldsymbol{\delta}^{\mathbf{x},l+1}) \odot \varphi'(\mathbf{z}^{\mathbf{x},l})$
  end for
end for
foreach $l \in L, L-1 \dots 2$ **do** ▷ ▷ Gradient descent
  $\mathbf{W}^l \leftarrow \mathbf{W}^l - \frac{\eta}{m} \sum_{\mathbf{x}} \boldsymbol{\delta}^{\mathbf{x},l} (\mathbf{a}^{\mathbf{x},l-1})^T$
  $\mathbf{b}^l \leftarrow \mathbf{b}^l - \frac{\eta}{m} \sum_{\mathbf{x}} \boldsymbol{\delta}^{\mathbf{x},l}$
end for

4 Results

The results starts with the problem definition and continues with what you have done. Try to give an intuition first and describe everything with words and then be more formal like 'Let g be ...'.

4.1 Problem Definition

Start with a very short motivation why this is important. Then, as stated above, describe the problem with words before getting formal.

4.2 First Part of the Results

4.3 N-th Part of the Results

5 Conclusion

Bibliography