INF203 - Advanced Programming Project

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1 Introduction

1.1 Group composition and responsibilities

1.2 Shared repository and tools for collaboration

1.3 Agile methodology and requirements analysis

1.4 User guide

2 Implementation

2.1 Code and Class Structure

2.2 Commenting

2.3 Advanced OOP techniques

In the Box class, we used Python's @property decorator to use the Box object easier and safer. Examples are shown in Figure 1.

```python
@property
def num_molecules(self):
    """Return the number of molecules in the box."""
    return len(self._molecules)

@property
def molecules(self):
    """Return a copy of the molecule list to prevent external
    modifications.
    """
    return self._molecules.copy()

@property
def dimensions(self):
    return (self._Lx, self._Ly, self._Lz)
```

Figur 1: How decorator @property is used in the class Box.

This techniques encapsulates the internal data and narrow down lines of code sometimes.

2.4 Python package

3 Functionality and validation

3.1 Testing and Validation Strategy

3.2 Initial Configuration Setup and Input/Output

3.3 Pair potential and Monte Carlo method

3.4 Test Area Method and Surface Tension Calculation

4 Sampling and data analysis

4.1 System Equilibration and Production

4.2 Uncertainty analysis, including Flyvbjerg-Petersen method

4.3 Data processing for console output

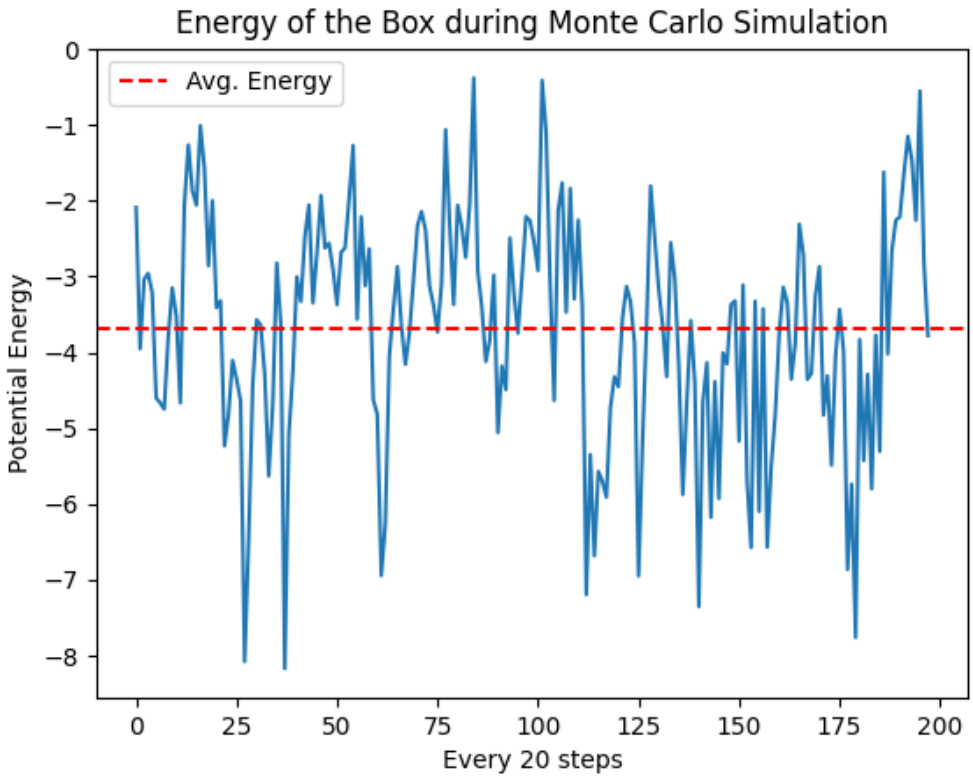
4.4 Data processing for diagrams and visualization

5 Simulation results

5.1 Vapour-only reference system

Question: What if you fill the complete box with gas? You can keep the compartments as they were and set the density to 0.02 everywhere.

Answer: When the density of the box become 0.02, which makes less molecules found the box than the reference scenario (molecules). Thus with keeping the same dimension of the box, the distance between molecules is likely to be farther so the initial total potential is pretty small, negative values near zero. Through Monte Carlo steps and towards the equilibrium, the average potential energy is a weak negative, shown as red line of value -3.68 units in figure 2. The convergence of this scenarios was noticeably fast.

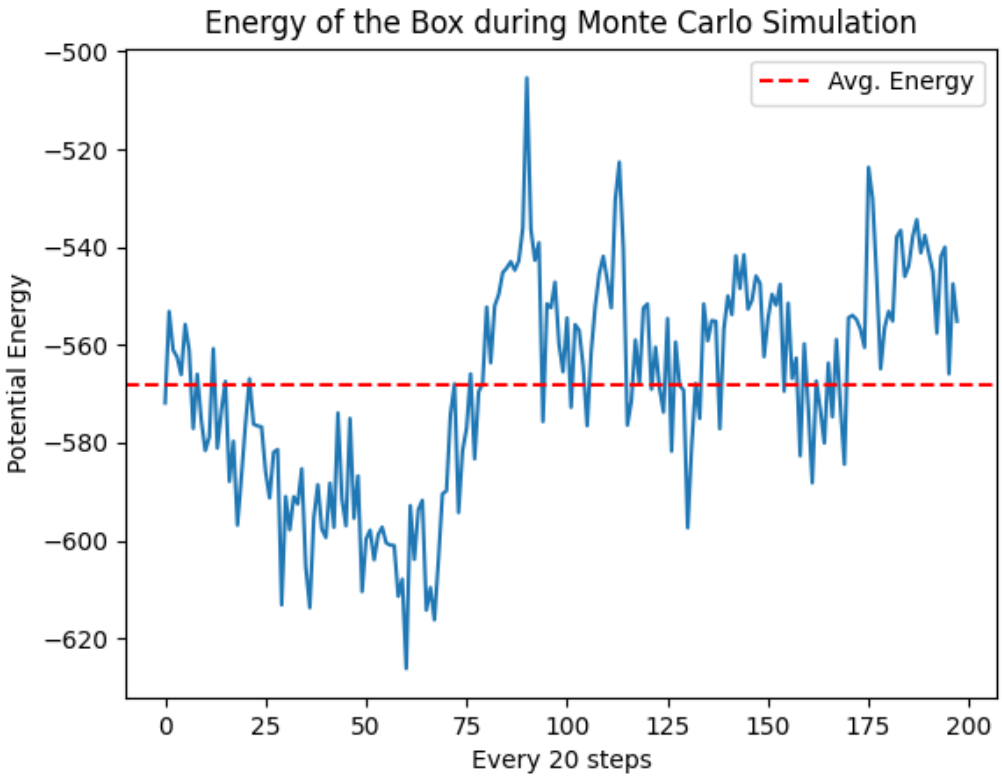


Figur 2: The Potential Energy of the Box only containing vapor over 10000 Monte Carlo steps.

5.2 Vapour-liquid reference system

Question: What potential energy do you find for the reference scenario from the first worksheet, with ρinit = 0.73, ρinit = 0.02, V = 5 × 40 × 5, and T = 0.8?

Answer: With this configuration, the number of molecules in the box amounts to 162 molecules. At the initial state, the total potential energy is typically very high and positive because the randomly generated molecules could lie very close to each other and some even overlaps. As the Monte Carlo steps move particles, the potential drops significant, observed with 10 steps frequency or lower. But after the third, fourth output records, the energy fluctuates around -500 to -600 units, which shows a negative realistic equilibrium state of energy (average of -568.2 units, shown as red line in figure 3). The negative sign of the interaction relfects the net attraction between molecules in the box.



Figur 3: Caption

5.3 Any other results

5.4 Comparison to results from the literature