Molecular dynamics

Introduction

- Molecular Dynamics is a computational method used to study the time-evolution of a set of interacting particles under the influence of classical mechanics.
- The simulation is based on the numerical integration of the equations of motion.
- In this presentation, we will explain the code for simulating Lennard-Jones particles, which are commonly used to model atoms or molecules in condensed-phase systems.

Code Explanation

- The code is written in Python, and it uses several libraries such as NumPy and Matplotlib.
- The simulation is performed by iterating over a fixed number of steps, where each step consists of four main functions: initialising positions and velocities, calculating forces, updating positions, and updating velocities.
- The simulation also includes a thermostat that adjusts the particle velocities to maintain a constant temperature.

The Simulation

- The simulation is based on the Lennard-Jones potential, which models the interactions between particles in a system.
- The simulation is performed in a cubic box of length lx=ly=lz=20 containing n_particulas=729 particles.
- The parameters for the Lennard-Jones potential are sig = 1 and ep = 0.4.
- The simulation runs for n_pasos=50000 steps with a time step of dt=0.005.

Initializing Positions and Velocities

- The inicializar_posiciones() function initialises the particle positions in a face-centred cubic lattice.
- The inicializar_velocidades() function initialises the particle velocities by assigning random values within a certain range.

Calculating Forces

- The calcular_fuerzas() function calculates the forces between particles using the Lennard-Jones potential.
- The function uses a neighbour list to reduce the computational cost of calculating the forces between distant particles.
- The energy and force contributions are truncated beyond a cutoff radius rc=2.5*sig.

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Updating Positions and Velocities

- The actualizar_posiciones() function updates the particle positions using the Verlet algorithm.
- The function applies periodic boundary conditions to simulate an infinite system.
- The actualizar_velocidades() function updates the particle velocities using the Verlet algorithm and the forces calculated in calcular_fuerzas().

Thermostat

- The Thermostat() function adjusts the particle velocities to maintain a constant temperature.
- The function rescales the velocities to achieve a target kinetic energy.

Results

- The simulation results are visualised using Matplotlib.
- The particle positions are plotted at the beginning and end of the simulation.
- The particle velocities are used to colour the final positions in a scatter plot.
- The temperature of the system is calculated from the kinetic energy and plotted as a function of time.

Conclusion

- The presented code provides a simple example of molecular dynamics simulation.
- The simulation can be extended to include more complex systems and interactions.
- The results obtained from the simulation can provide insight into the dynamics of a wide range of systems, from materials to biological molecules.

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[Introduction]

The modelling of intermolecular interactions is an important goal in theoretical physics. The thermodynamics of a fluid can be obtained using statistical mechanics if the potential function describing the interaction between molecules is known.
In this study, we focus on modelling intermolecular interactions in a cluster of argon atoms using the Lennard-Jones (LJ) potential. We perform molecular dynamics simulations using Python, a popular language with numerous freely available libraries.
The LJ potential has been used extensively due to its simplicity and ability to produce physically acceptable results. It has also been used to model non-polar substances.
The LJ potential was initially proposed by J. Lennard-Jones in 1931, and its form was deduced by F. London in 1930. One of the first computer simulations using this model was performed by Wood and Parker in 1957.
The main goal of this study is to analyse the properties of the Lennard-Jones potential and its ability to model interatomic interactions in argon molecules. We perform molecular dynamics simulations of the argon cluster and study the behaviour of the potential energy and potential energy curve for 729 particles.

[Theoretical framework]

The LJ potential describes the interaction between two atoms in terms of a repulsive and an attractive component. It can be expressed as a function of the distance vector between the atoms, the size of the particle at which the intermolecular potential between two atoms is zero, and the depth of the potential well.
LJ potential has been extensively reviewed, using methods such as molecular dynamics, X-ray diffraction, and microwave spectroscopy, to determine the parameter values.
The LJ potential has a minimum value when the interatomic force is zero. Reduced units are used to perform molecular dynamics simulations.
The Velocity-Verlet algorithm is used to simulate the motion of particles in molecular dynamics. The Verlet velocity algorithm is stable and accurate, making it suitable for simulating complex and highly dynamic systems.
To maintain a constant temperature during the simulation, a thermostat is used to adjust the velocities of the particles at each iteration of the algorithm.

[References]

Several other models have been proposed to describe interatomic interactions besides the LJ potential, such as the Morse model and the Buckingham model.
The choice of the repulsion exponent in the LJ potential has been shown to improve the accuracy of molecular dynamics simulations.
Some authors have reported computational errors that can cause deviations in results.

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Discussion

- The Lennard-Jones potential is a widely used model for simple fluids, describing intermolecular interactions through the depth of the potential well and the distance at which the potential energy is zero.
- Python is a popular language for scientific computing, with many freely available libraries.
- The main goal of this study was to model interatomic interactions in argon clusters using the Lennard-Jones potential and investigate the potential's ability to produce physically accurate results.
- The initial state of the system has a significant impact on simulation results, and using random number generators with uniform distributions for initial positions can prevent simulation failures.
- Future studies could explore the inclusion of long-range interactions or the simulation of non-spherical particle systems.

Conclusion

- The behaviour of an argon particle system was simulated using the Lennard-Jones potential, and the effects of temperature and density on particle motion were studied.
- The choice of initial system state significantly affects simulation results, and using random number generators with uniform distributions for initial positions can prevent simulation failures.
- Future studies could explore possible extensions, such as the inclusion of long-range interactions or the simulation of non-spherical particle systems.

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