Documentation and User Guide

Molecular Dynamics Program for Argon

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1 The program

This project contains a program for running molecular dynamics (MD) simulations for Argon. The program reads atomic coordinates and masses from an input file and performs a MD simulation using the Verlet algorithm and the Lennard-Jones potential. The trajectory in XYZ format, as well as an extended trajectory file including velocities, the accelerations and energies for each step are generated as output.

2 Installation

2.1 Prerequisites

Ensure you have the following installed on your system.

```
gcc
make
```

2.2 Installation

1. Clone the repository:

```
git clone https://github.com/pauline-schtt/tccm-homeworks/tree/master/project3
cd project3
```

2. Compile the program using `make`:

```
make
```

3. Then, run the program:

```
./MD <path_to_the_input_file>
```

Installation instructions can also be found in the `INSTALL.md` file.

3 Usage

To run the molecular dynamics simulation, provide the full path to the input file containing the atomic coordinates and masses as an argument to the program. An example input file can be found in `data/inp.txt`.

Example:

```
./MD data/inp.txt
```

4 Input format

Atomic coordinates are provided in nm in the following format:

```
<number of atoms>
<x_1>   <y_1>   <z_1>   <mass_1>
<x_2>   <y_2>   <z_2>   <mass_2>
...
<x_n>   <y_n>   <z_n>   <mass_n>
```

Example:

```
3
0.0   0.0    0.0   39.948
0.0   0.0    0.5   39.948
0.1   0.2   -0.5   39.948
```

An example input file can be found in the `data` folder.

5 Output format

The program produces the following output files:

- **trajectory.xyz**: atomic coordinates for each step of the simulation in XYZ format, kinetic, potential and total energy are provided on the comment line
- **trajectory_velocities.xyz**: similar to trajectory.xyz, but additionally contains the velocities for each atom
- **energies**: kinetic, potential and total energy for each step of the simulation
- **accelerations**: acceleration in x, y and z direction for each atom for each step of the simulation

The trajectory in XYZ format can be opened and visualized, e.g. with the VMD or JMOL software.

Example output files can be found in the `tests` folder.

6 Default values

The program uses the following default values:

- number of steps: 1000
- time step: 0.2
- mass of Argon: 39.948 g/mol
- ϵ: 0.661 j/mol
- σ: 0.3345 nm

Velocities are initialized to zero.

No thermostat is used, but conversation of the total energy is checked at each step and the user is warned if the energy varies significantly.

7 Tests

The program was tested on MacOS Sequoia 15.2 and Ubuntu 24.04. You can find an example input file in the `data` folder, while the corresponding output files can be found in the `test` folder. As no random velocity initialization is performed, you should obtain qualitatively similar results when running the program with the test input.

8 Cleaning up

To clean up the compiled files, run:

```
make clean
```

9 Troubleshooting

If you encounter any issues during the installation, ensure that your versions of the prerequisites meet the required versions mentioned above. In case you're still facing issues, feel free to reach out to any of the contributors or opening an issue on GitHub.

10 License

11 Acknowledgments

This project is based on data and instructions provided by Abdallah Ammar, Yann Damour, Peter Reinhardt and Anthony Scemama, available at https://github.com/scemama/tccm-homeworks.

Appendix

Detailed documentation on the file contents, functions and variables in the code are provided in the documentation as generated using Doxygen (https://www.doxygen.nl/) in the appendix.