User Manual (MDS)

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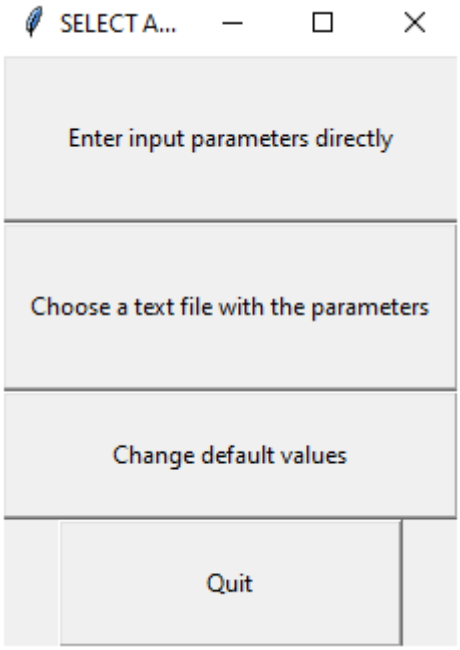
1. Starting the application

There is a file named “Main.py” which shall be executed

2. Graphical User Interface

Once the application has been opened, it will display the next window



“Enter input parameters directly” allows the user to write down in a different window all the parameters that the simulation is able to run.

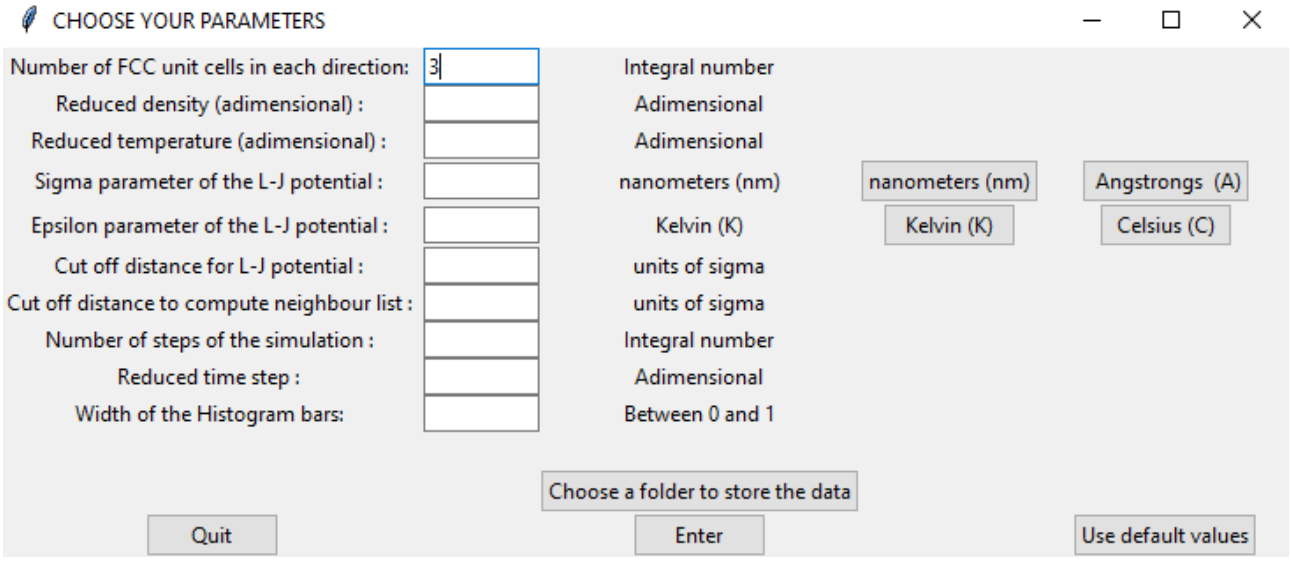
“Choose a text file with the parameters” allows the user to select a text file with all the parameters.

“Change default values” if some parameters are missing, the system will run some default values. This button allows the user to change them by writting them down.

“Quit” Close the window and stops the application.

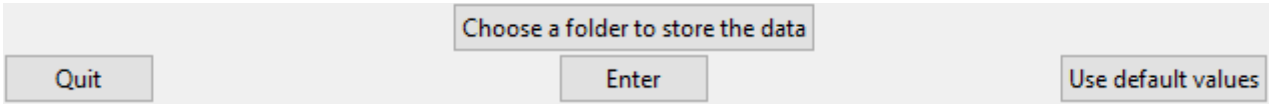
2. 1. Enter input parameters directly

If the user select the first option (Enter input parameters directly), the following window will be displayed



We can see 10 text boxes, where the user is able to write the different parameters that the simulation is able to run. Each box has at the left the definition of the parameter and at the right, the units that the program is using. The user can change some of the units by clicking on the buttons.

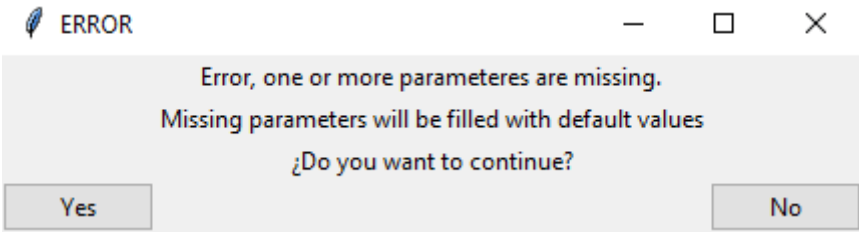
At the bottom of the window, we can see 4 buttons.



“Quit”: Close the window and stops the application

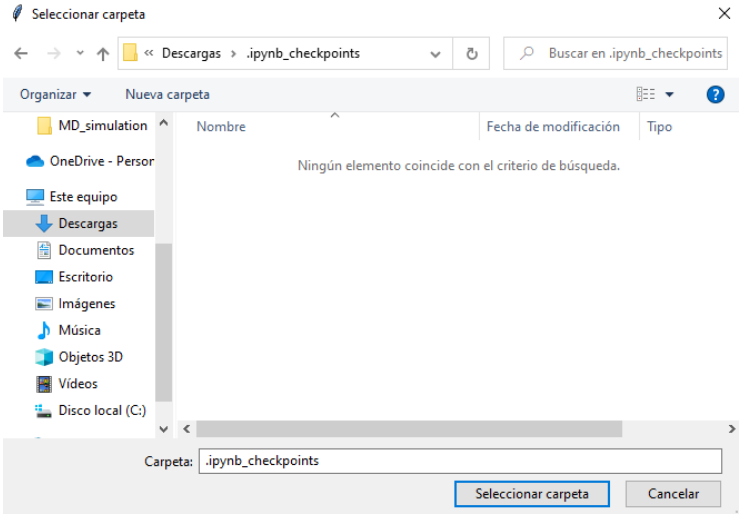
“Use default values”: Start the simulation with the default values stored, it will not use any of the box values.

“Enter”: Starts the simulation with the given values, if some of them are missing, the application will tun this window



If the user press “Yes” the simulation will start with the values from the boxes and the boxes with parameters with no value will be running with their corresponding default value.
If the user press “No” the error window is closed and the user will be able to write the rest of the parameters

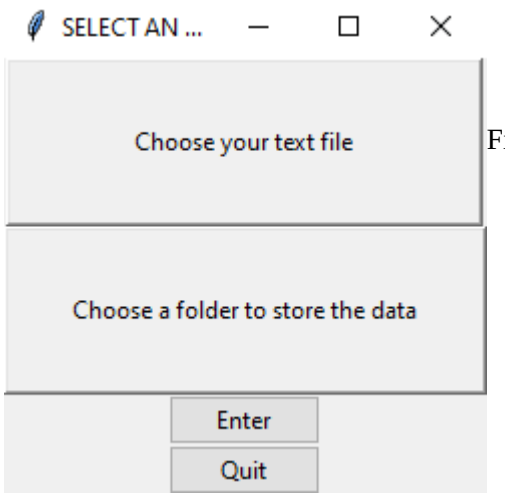
“Choose a folder to store the data” Display this kind of window



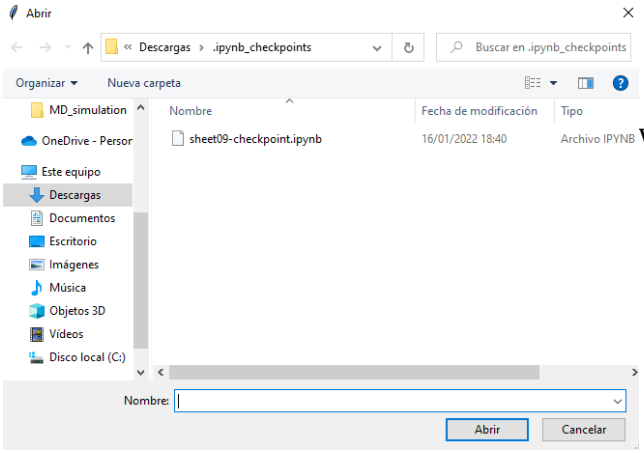
And allows the user to select a specific folder to store all the data computed by the simulation.

2. 2. Choose a text file with the parameters

This option allows the user to input the parameters stored in a text file.



First option, “Choose your text file” display the next window



Where the user can select a text file with the parameters.

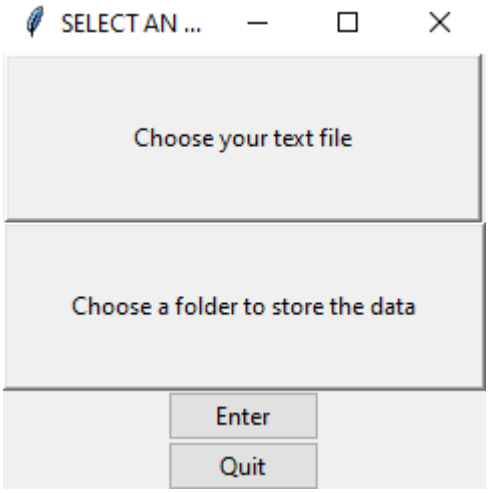
The format of the text file must be the next one

```
NumberFCCUnits      3

ReducedDensity      0.8442
ReducedTemperature  0.722
Sigma               0.341 nm
Epsilon             119.8 K
CutoffPotential     2.5

CutoffList          2.7

NumberOfSteps       3
ReducedTimeStep     0.005
WidthBinPairDistributionFunction 0.1
```

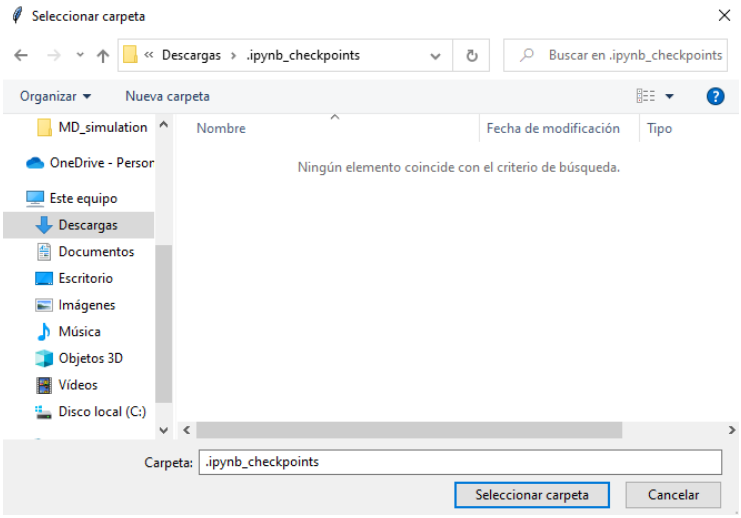
Number of FCC unit cells in each direction in the supercell.

Reduced density (adimensional).
Reduced temperature (adimensional).
Parameter sigma of the Lennard-Jones potential.
Parameter epsilon of the Lennard-Jones potential.
Cutoff distance for truncation of intermolecular potential. (in units of sigma).
Cutoff distance for the computation of Verlet neighbor list (in units of sigma).
Number of steps in the Molecular Dynamic simulations.
Reduced time step.
Width of the bins in the histogram to compute the pair distribution function.

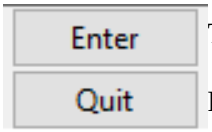
The specific name of the parameter is in the first column and must be in the same as the one showed in the figure, followed by the number. The order of the parameters is not relevant. The file must contain this 10 parameters and the units of “Sigma” (“nm” = nanometers, “A” = Angstroms) and “Epsilon” (“K”= Kelvin, “C” = celsius).



Second option , “Choose a folder to store the data” allows the user to select a specific folder where all the data computed will be stored. It will display the following window.



And allows the user to select a specific folder to store all the data computed by the simulation.

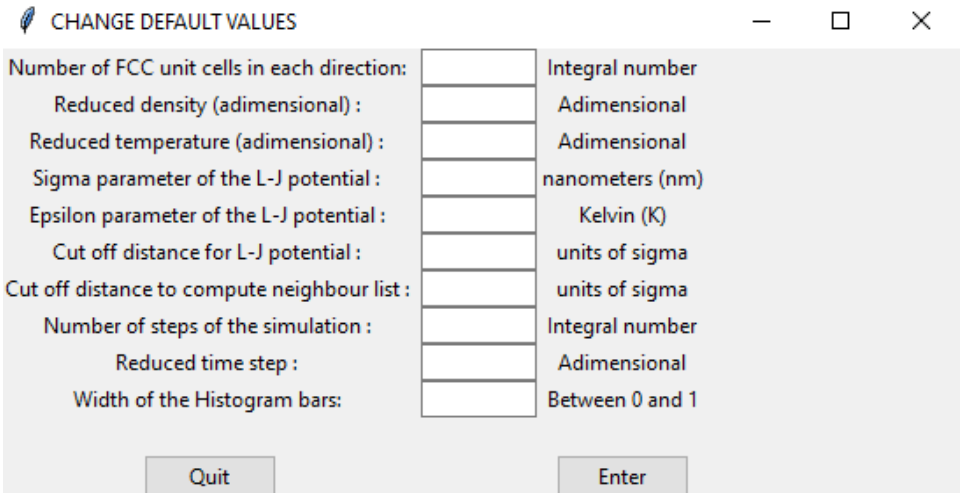


Third option “Enter” starts the simulation with the selected options in buttons 1 and 2.

Forth option “Quit” close this windows and stops running the application.

2. 3. Change default values

This option allows the user to change the default values of the simulation, by selecting this option the application displays the next window



The window contains 10 text boxes where the user can write down the different parameters. At the left of the box is specified the parameter and at the right the units used. Text boxes that are not filled, will not change.

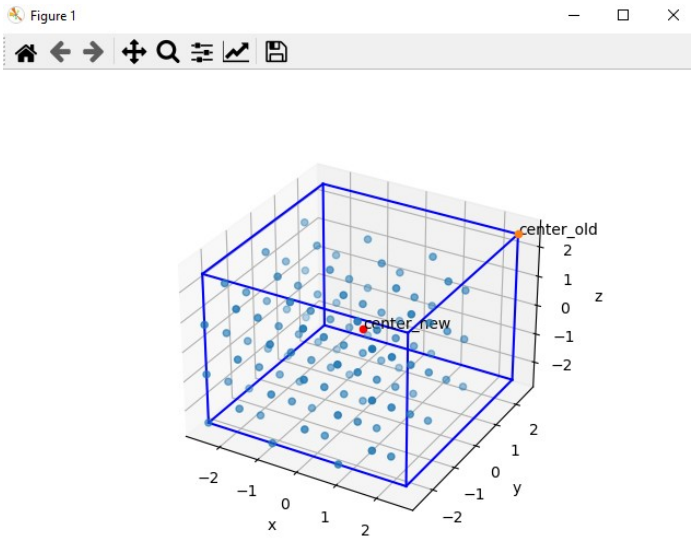
“Quit” button close this window and stops running the application and “Enter” close the window but saving all changes done in the default values.

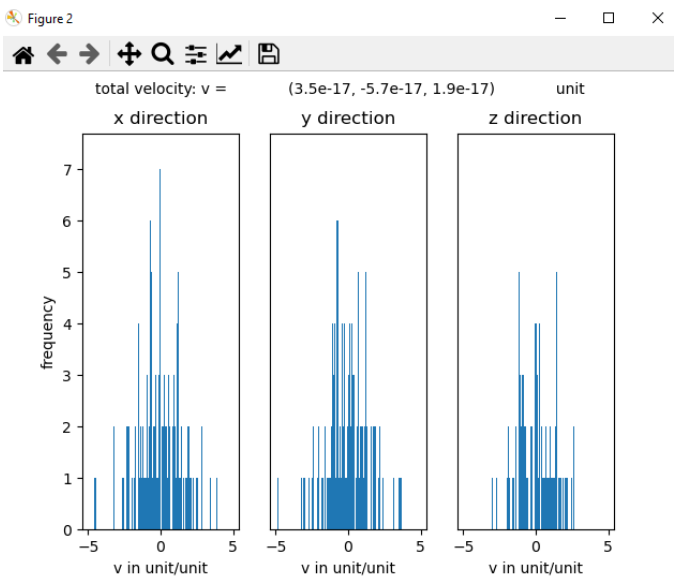
3. Returns

Once the user has introduced the parameters, the simulation is initialized and provides the user different data at the starting and at the end of the simulation.

3. 1. Displays

At the starting of the simulation, the application shows two images, first one is a 3 Dimensional plot of the initial positions of the atoms, including the simulation box, and second one is a histogram of velocities in the 3 dimensions (x, y, z).



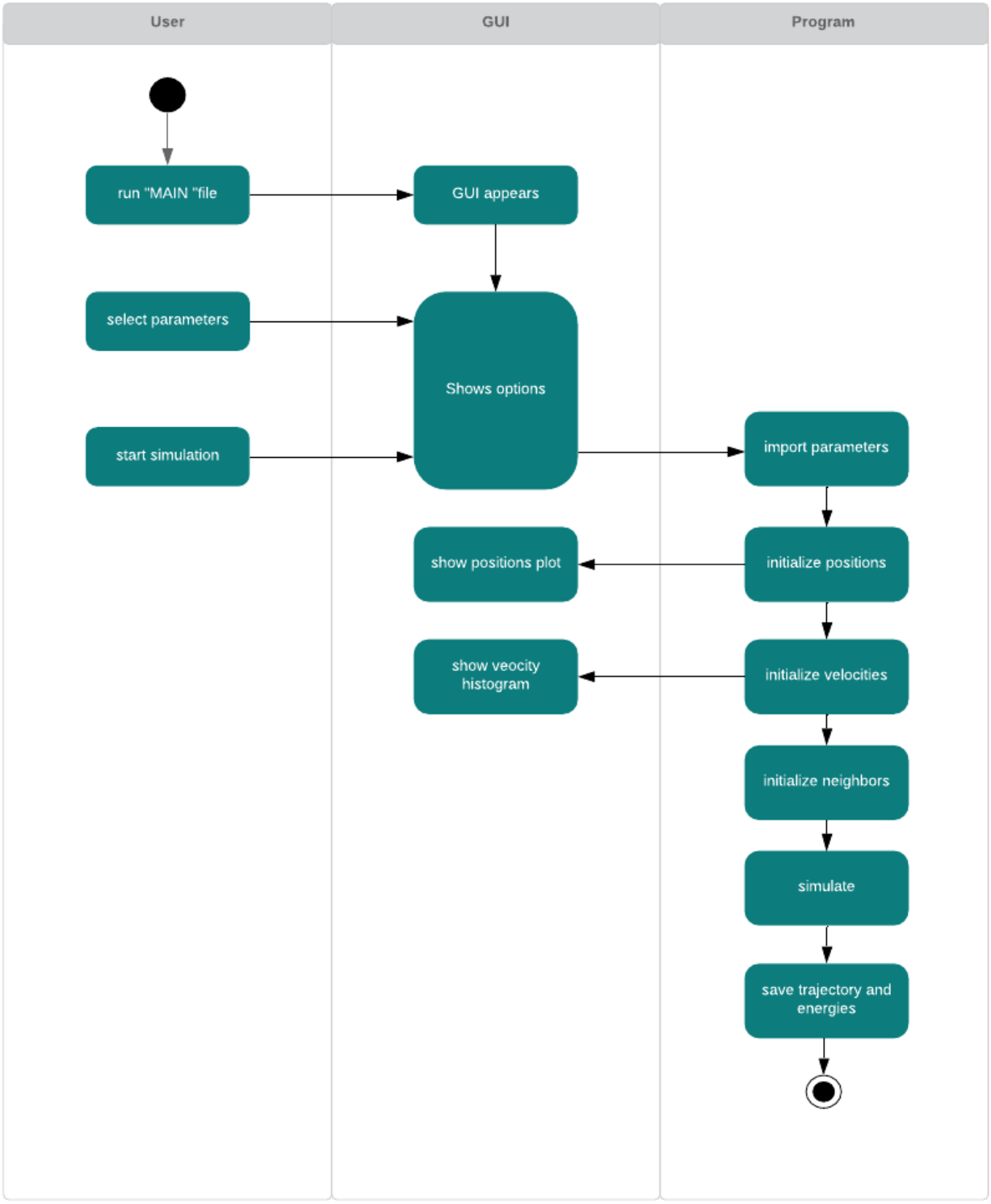


This figures can be examinated and saved.

3. 1. Data

The remaining data of the simulation is saved in the selected that the user has specified before. In case that there is not such directory the data will be stored in the same directory as the application.
This data is stored in text files. First file stores all the initial coordinates (x, y, z) for each atom index. Second one contains every atom initial velocity in every direction (x, y, z) for it specific atom index. Third one is the initial neighbor list used to compute the Verlet algorithm, it contains the index and the position of the atom followed by the index and positions of the rest of the atoms. Forth file is provided at the end of the simulation and contains all the trajectories of the atoms for every time step of the simulation. Fifth file is also given when the simulation is finished and stores the total energy of the system (potential, kinetic, and the summation of both) for every time step.

4. Sequence diagram



5. Miscellaneous

The history of this project can be found under https://github.com/emil-ho/AdvancedComputation
Through vectorization of several for loops, the simulation runs a lot faster than with the loops. For the final version it was only partially possible to use vectorized versions of the functions. Because of this, a version without neighbor list is actually faster, but the difference gets smaller for more Atoms.