

Molecular dynamics simulation

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Requirement list

1. Input/output
2. Initialization
3. Neighbour list
4. Potential, energies and forces
5. Integration of Newton's 2nd law

Requirement list

1 INPUT/OUTPUT:

- 1.1 Data from an input text file
- 1.2 No order in the input file
- 1.3 Different system of units
- 1.4 Default values for the parameters
- 1.5. A GUI

2 INITIALIZATION:

- 2.1 Initial positions of FCC lattice
- 2.2 Maxwell-Boltzmann distribution for V_i
- 2.3 Initial positions in a file
- 2.4 Initial velocities in a histogram

Requirement list

3 NEIGHBOUR LIST:

- 3.1 Verlet's neighbour list
- 3.2 Initial neighbour list in a file

4 POTENTIAL, ENERGIES, AND FORCES:

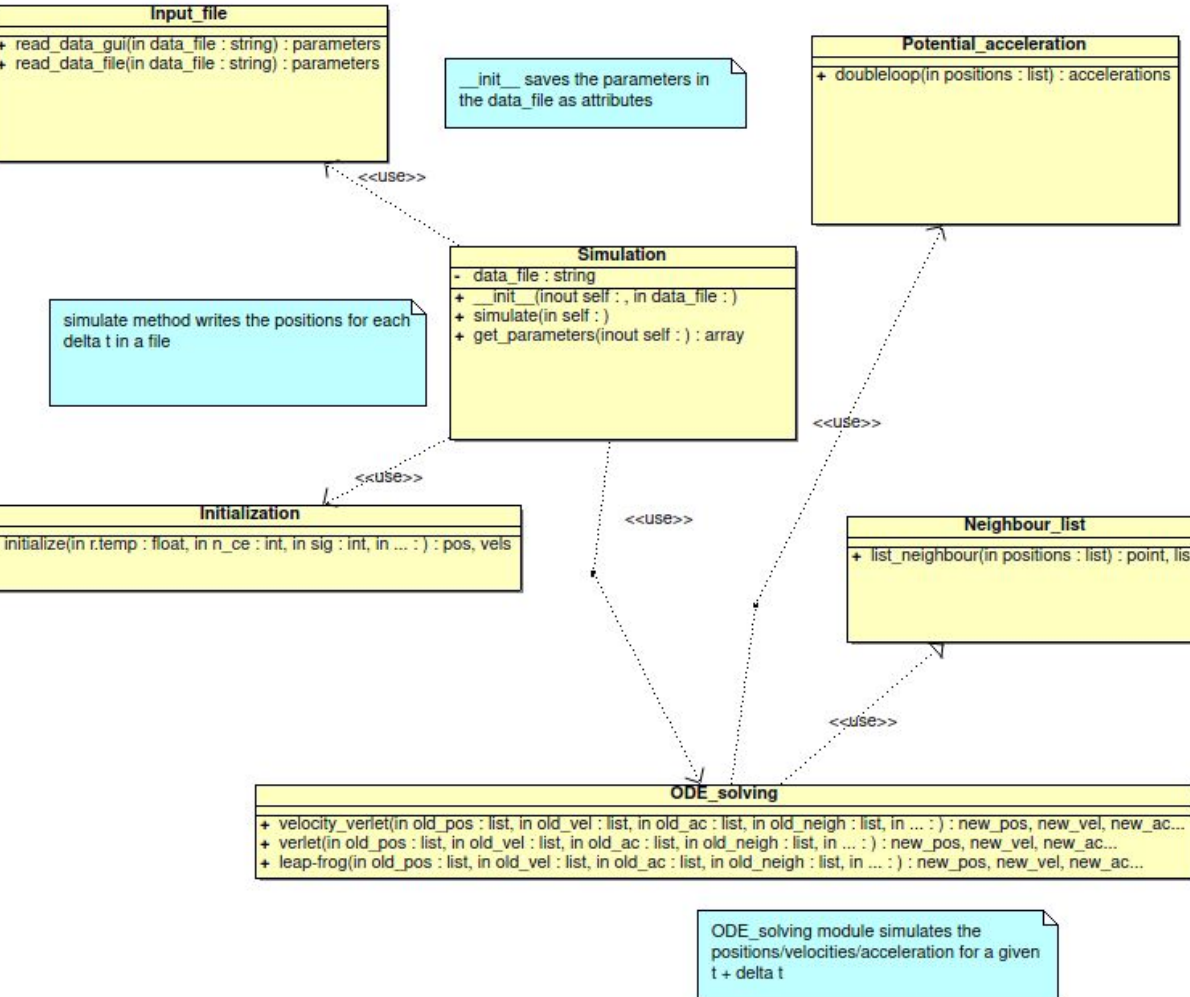
- 4.1 Shifted Lennard-Jones potential
- 4.2 Energies and temperature in a file
- 4.3 Original Lennard-Jones potential
- 4.4 GUI with type of potentials

5 INTEGRATION OF NEWTON'S 2nd LAW:

- 5.1 Verlet's algorithm
- 5.2 Positions in a text file
- 5.3 GUI with integration algorithms
- 5.4 Custom the integration algorithm

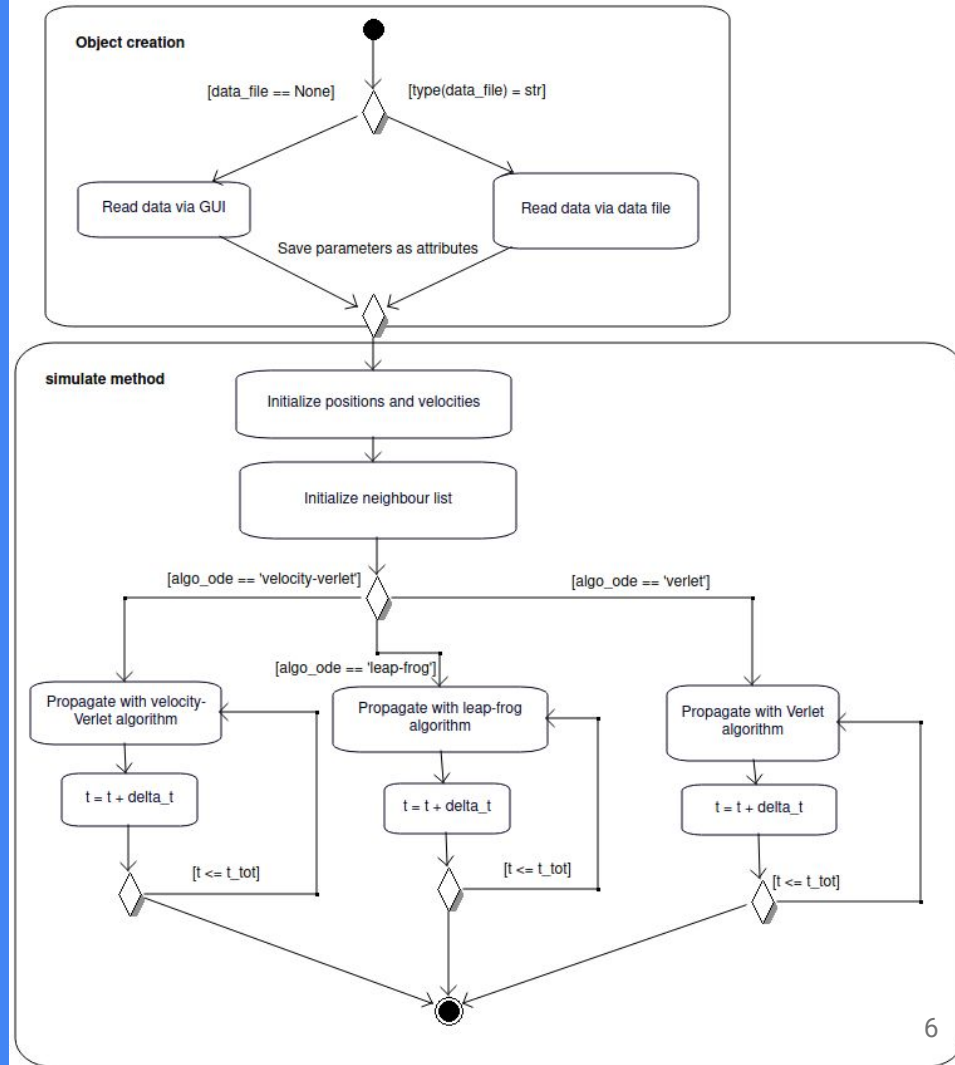
UML model

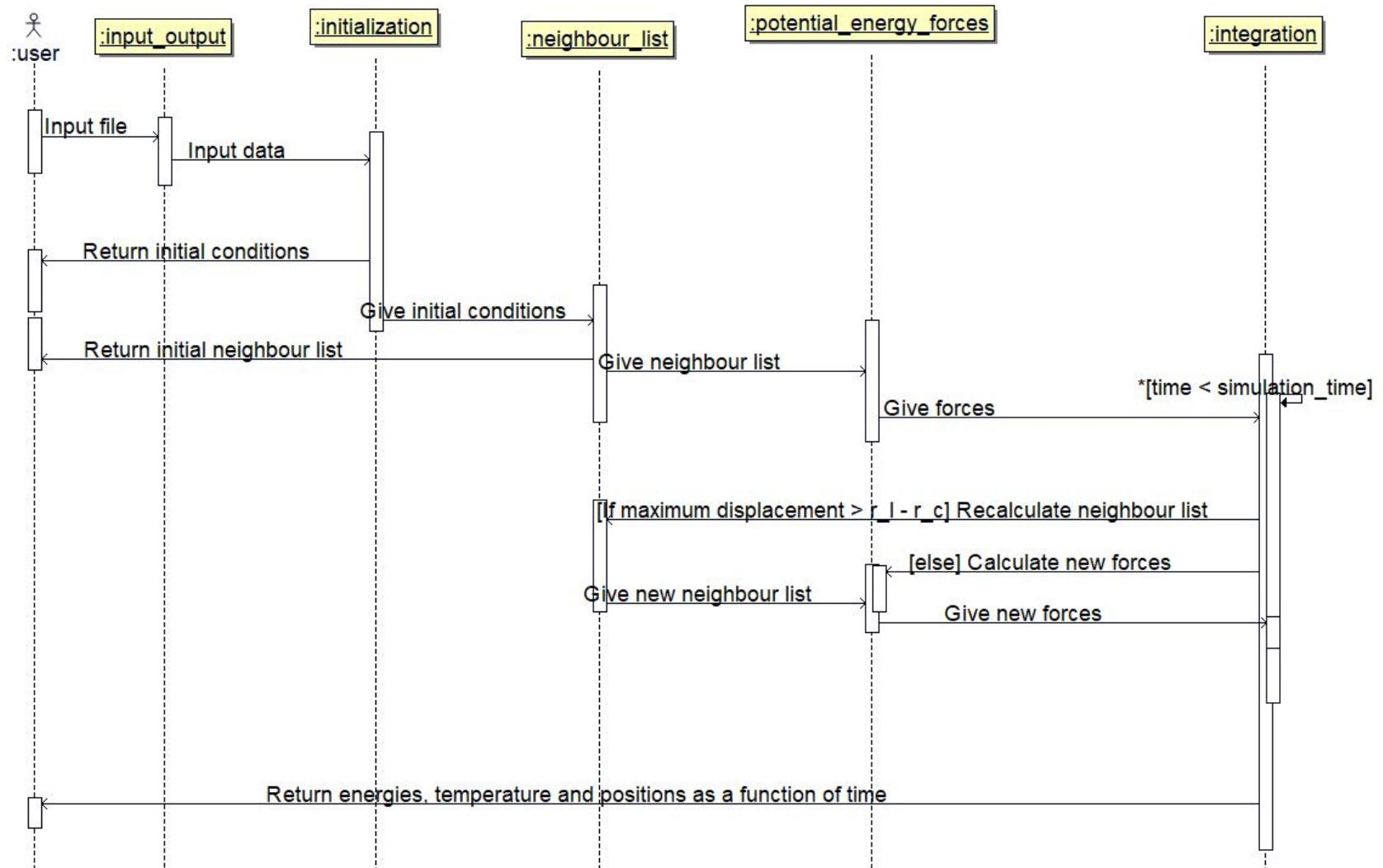
Schematic class diagram



UML model

Activity diagram of the object creation and the simulation method





Input: GUI

* Change to project folder:

cd Route_To_Project_Folder

- Command:

python run_simulation.py

- Alternative:

Double click in the
executable file *run.sh*

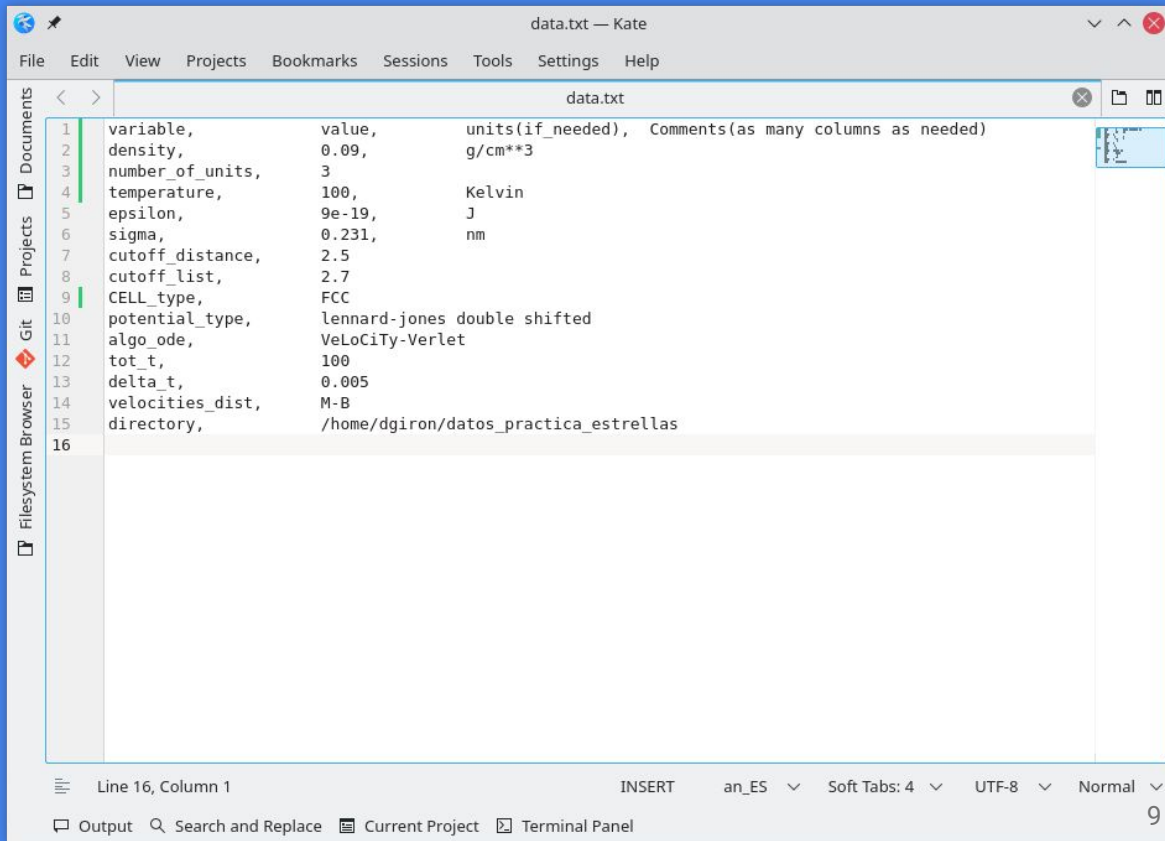
Input: data file

Command:

`python run_simulation.py`
`--data_file=FILE_NAME`

Command for help:

`python run_simulation.py --help`



```
data.txt — Kate
File Edit View Projects Bookmarks Sessions Tools Settings Help

data.txt
1 variable, value, units(if_needed), Comments(as many columns as needed)
2 density, 0.09, g/cm**3
3 number_of_units, 3
4 temperature, 100, Kelvin
5 epsilon, 9e-19, J
6 sigma, 0.231, nm
7 cutoff_distance, 2.5
8 cutoff_list, 2.7
9 CELL_type, FCC
10 potential_type, lennard-jones double shifted
11 algo_ode, VeLoCiTy-Verlet
12 tot_t, 100
13 delta_t, 0.005
14 velocities_dist, M-B
15 directory, /home/dgiron/datos_practica_estrellas
16

Line 16, Column 1
INSERT an_ES Soft Tabs: 4 UTF-8 Normal
Output Search and Replace Current Project Terminal Panel
```

Data file: error testing

Some of the error tests implemented include:

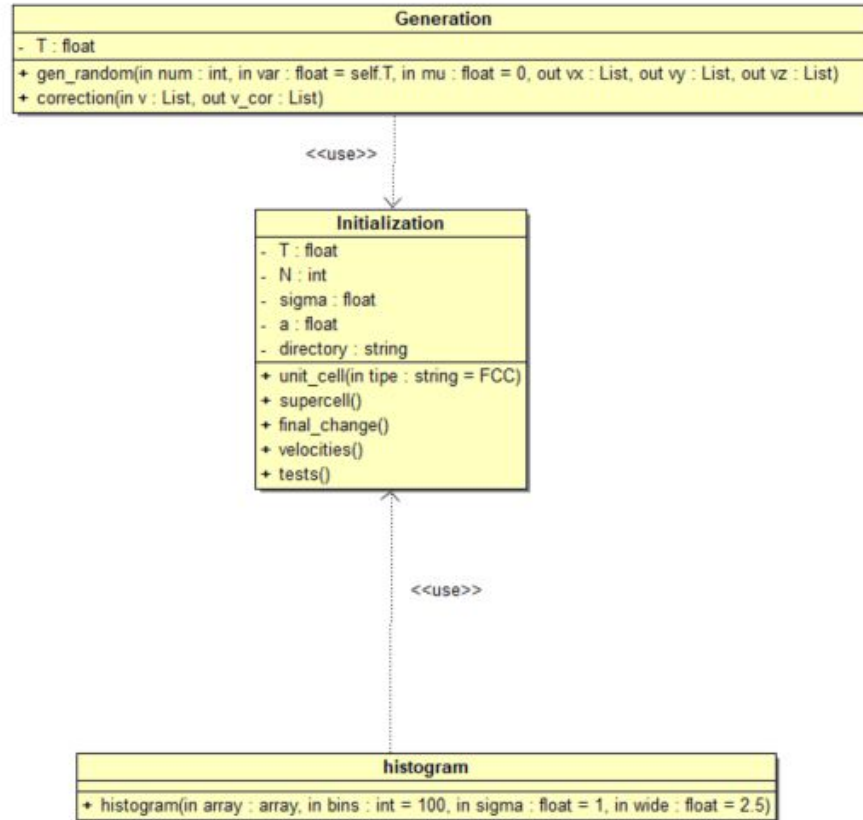
- Check if keyword correctly spelled
- Check if unit is admitted
- Check if there is any keyword missing
- Check if data file exists, if not it uses a default one

Data file: flexibilities

Some of the flexibilities implemented:

- Header row omission
- Capital letter use
- Order of keywords

Initialization: class diagram



Initialization: Output

$T=100$, $N=10$, $\sigma=2$, $a=0.1$

positions

velocity histogram

```
initial_positions.dat: Bloc de notas
Archivo Edición Formato Ver Ayuda
Initial position of the atoms in the supercell divided in unit cell
blocks in a system of units where sigma is 1 and the origin
is placed at the center of the supercell, in cartesian coordinates

1 [-0.25 -0.25 -0.25]
2 [-0.25 -0.225 -0.225]
3 [-0.225 -0.25 -0.225]
4 [-0.225 -0.225 -0.25 ]

5 [-0.2 -0.25 -0.25]
6 [-0.2 -0.225 -0.225]
7 [-0.175 -0.25 -0.225]
8 [-0.175 -0.225 -0.25 ]

9 [-0.15 -0.25 -0.25]
10 [-0.15 -0.225 -0.225]
11 [-0.125 -0.25 -0.225]
12 [-0.125 -0.225 -0.25 ]

13 [-0.1 -0.25 -0.25]
14 [-0.1 -0.225 -0.225]
15 [-0.075 -0.25 -0.225]
16 [-0.075 -0.225 -0.25 ]

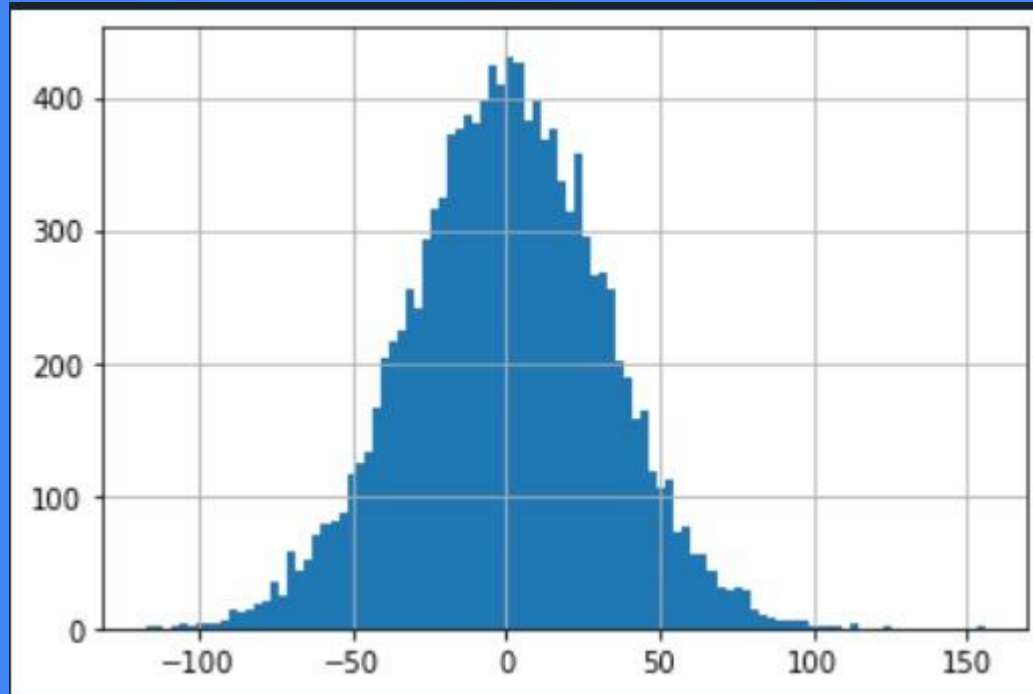
17 [-0.05 -0.25 -0.25]
18 [-0.05 -0.225 -0.225]
19 [-0.025 -0.25 -0.225]
20 [-0.025 -0.225 -0.25 ]

21 [ 0. -0.25 -0.25]
22 [ 0. -0.225 -0.225]
23 [ 0.025 -0.25 -0.225]
24 [ 0.025 -0.225 -0.25 ]
```

```
*velocity_histogram.dat: Bloc de notas
Archivo Edición Formato Ver Ayuda

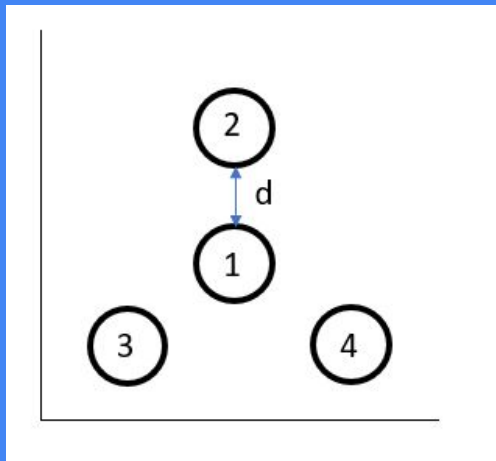
-90.000000000 7
-88.000000000 6
-86.000000000 6
-84.000000000 10
-82.000000000 9
-80.000000000 19
-78.000000000 21
-76.000000000 25
-74.000000000 17
-72.000000000 26
-70.000000000 43
-68.000000000 29
-66.000000000 35
-64.000000000 38
-62.000000000 42
-60.000000000 46
-58.000000000 56
-56.000000000 66
-54.000000000 61
-52.000000000 79
-50.000000000 101
-48.000000000 93
-46.000000000 119
-44.000000000 109
-42.000000000 135
-40.000000000 147
-38.000000000 162
-36.000000000 172
-34.000000000 186
-32.000000000 210
-30.000000000 188
-28.000000000 182
-26.000000000 232
-24.000000000 237
-22.000000000 219
-20.000000000 265
```

Distribution of velocities



Neighbour list

Without boundary conditions



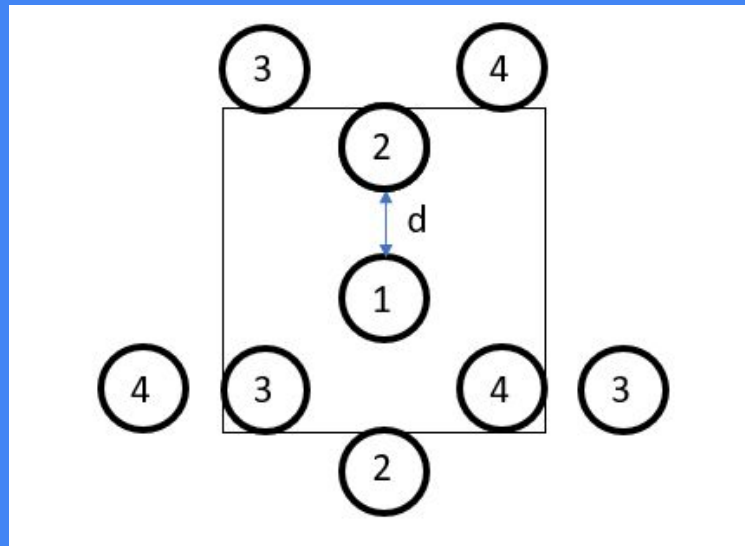
LIST

2	3	4	1	1	1
---	---	---	---	---	---

POINT

0	3	4	5
---	---	---	---

With boundary conditions



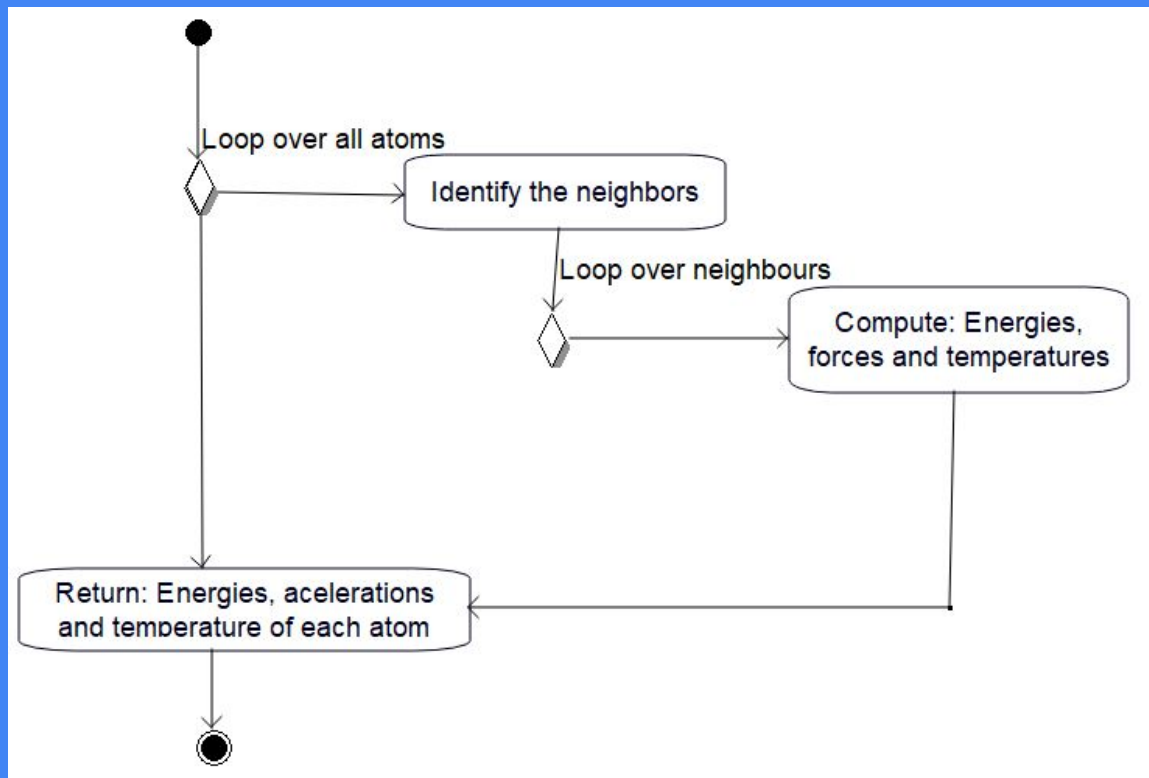
LIST

2	3	4	1	3	4	1	2	4	1	2	3
---	---	---	---	---	---	---	---	---	---	---	---

POINT

0	3	6	9
---	---	---	---

Potential energies and forces



ODE algorithms

- Activity diagram of the algorithm
- Essentially the same for every algorithm, just some small changes

