Molecular Dynamics Simulation for Lennard-Jones Pair Interaction

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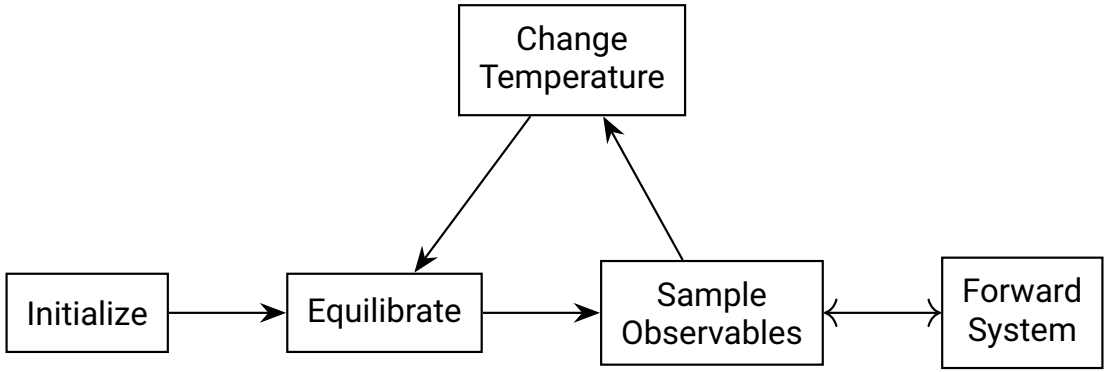
System

- Gas of classical particles interacting via Lennard-Jones (L-J) pairwise potential
- Simulation box is two-dimensional with periodic boundary conditions to mimic infinite system
- Number of particles & volume are fixed; temperature is varied to study different states
- Particles initialized with random velocities from Maxwell-Boltzmann distribution
- Goal is to simulate system in order to study certain thermodynamic properties.

Simulation

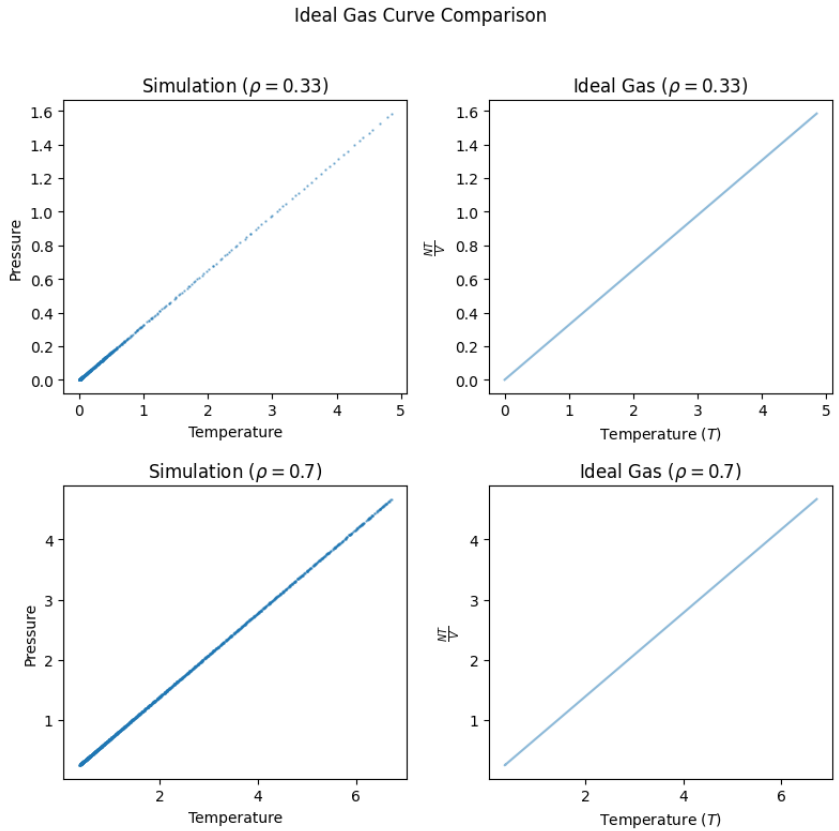
- Data structure for system information:
  - particle positions and velocities as lists of doubles
  - initial state
  - simplify boundary conditions
  - process for state evolution
- Force: shifted & truncated L-J potential
- Position/Velocity updating: velocity-Verlet

Data Capture



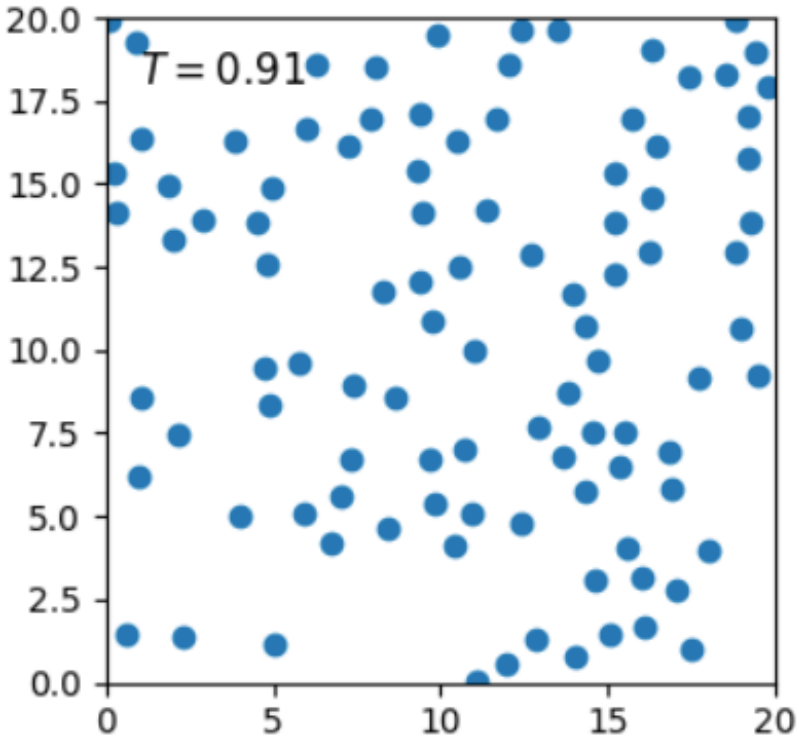
- Observables effectively get calculated during system forwarding anyway
- Change temperature by multiplying all velocities by the same double

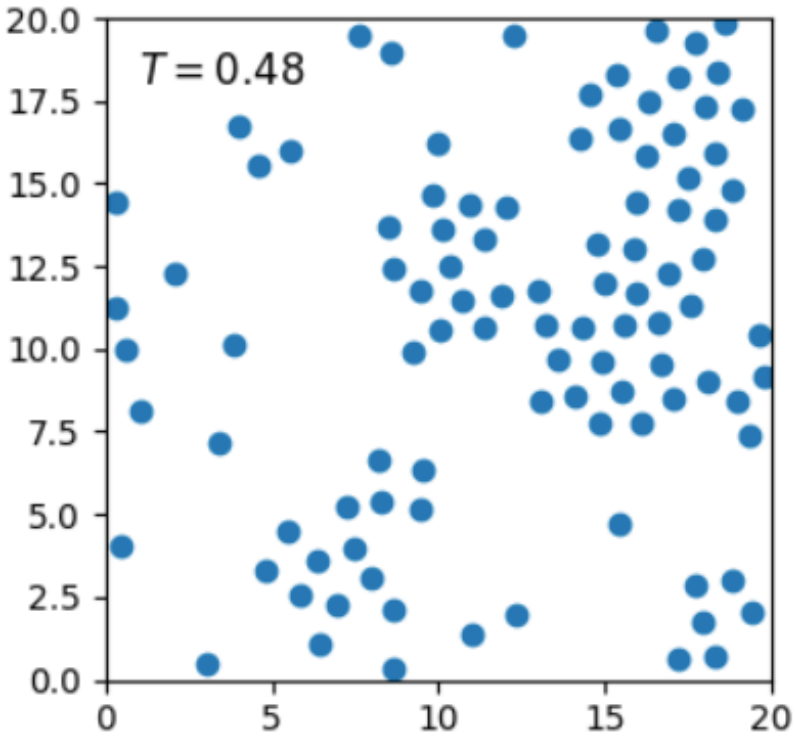
Data

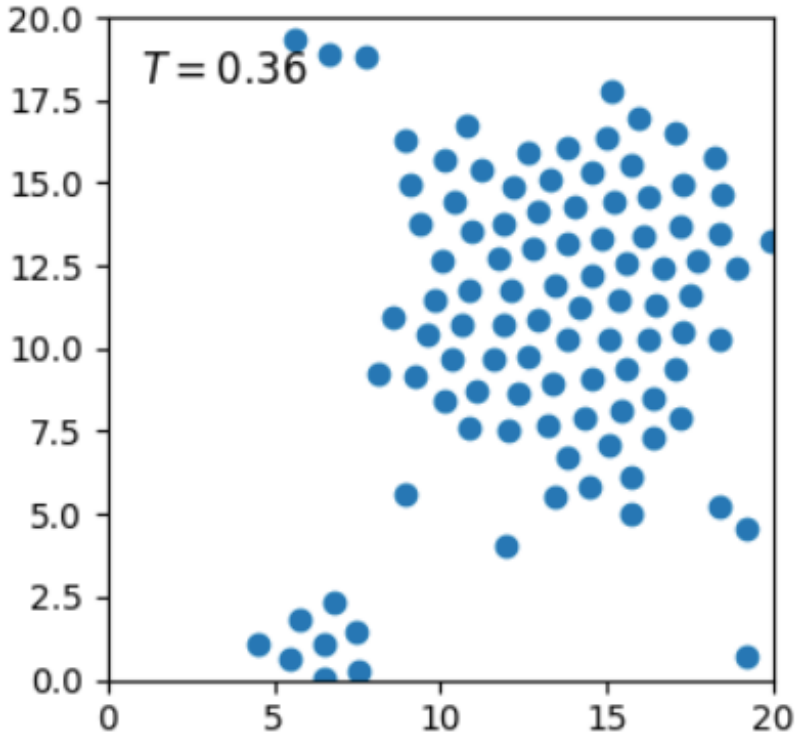


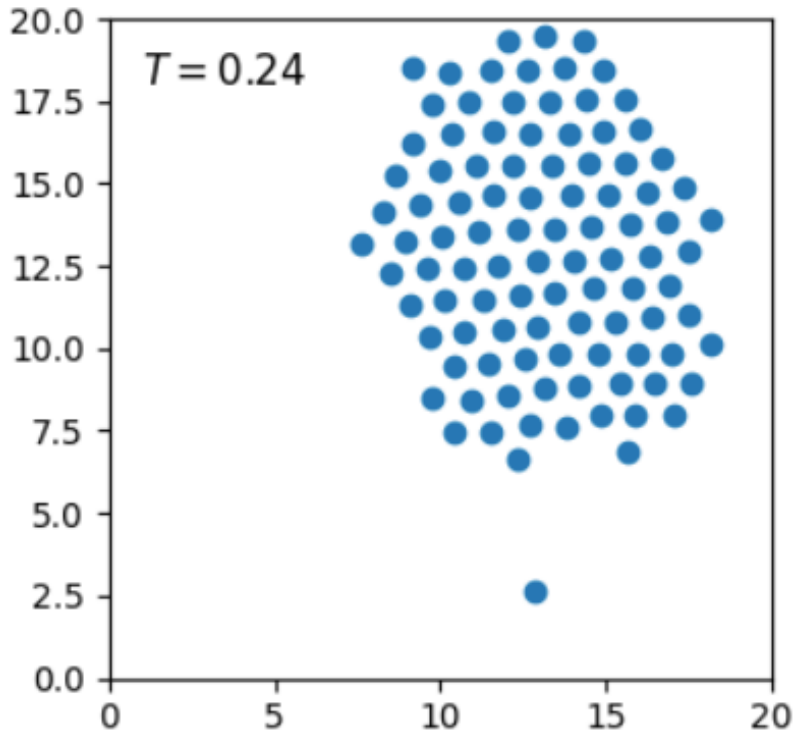
- Second term term contributes impulsively at higher temperatures

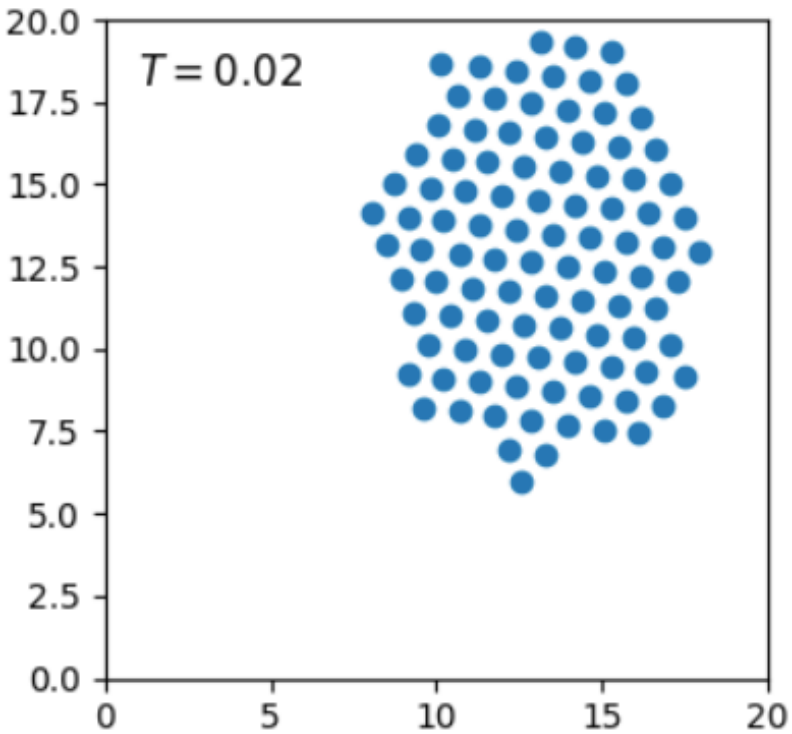
Effects of Temperature



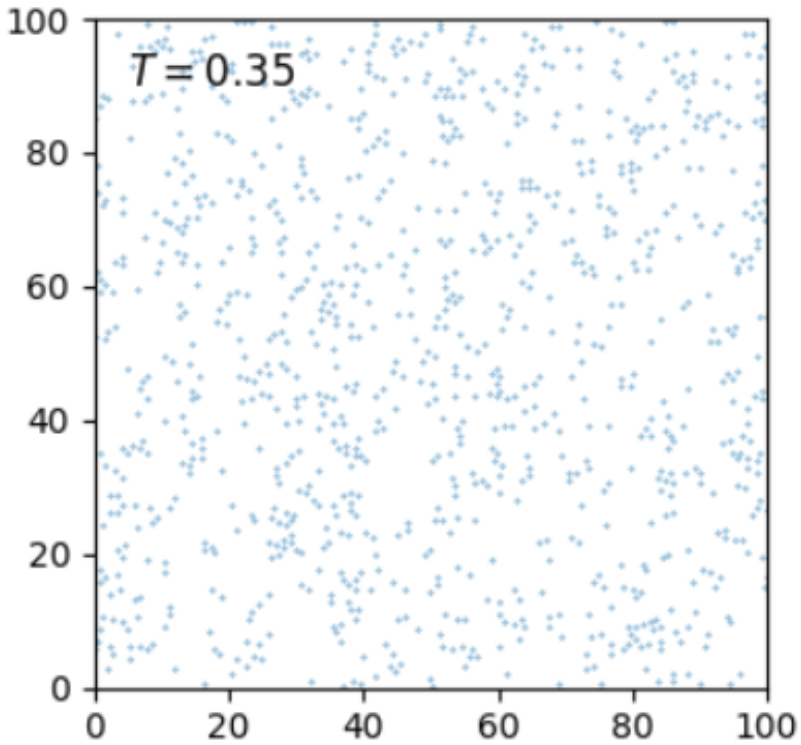

$T = 0.48$
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20

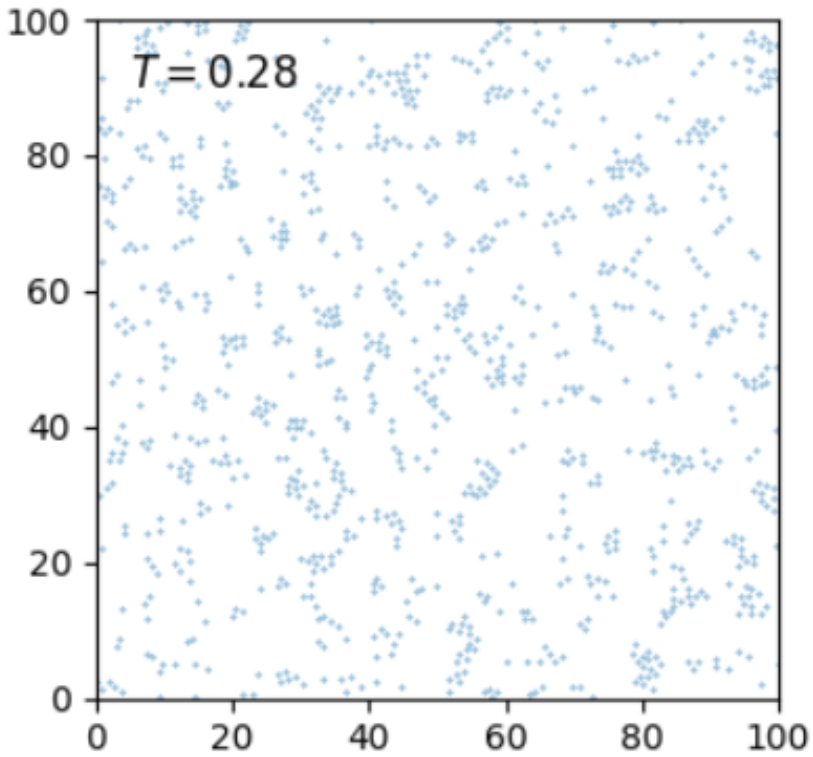

$T = 0.36$
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20

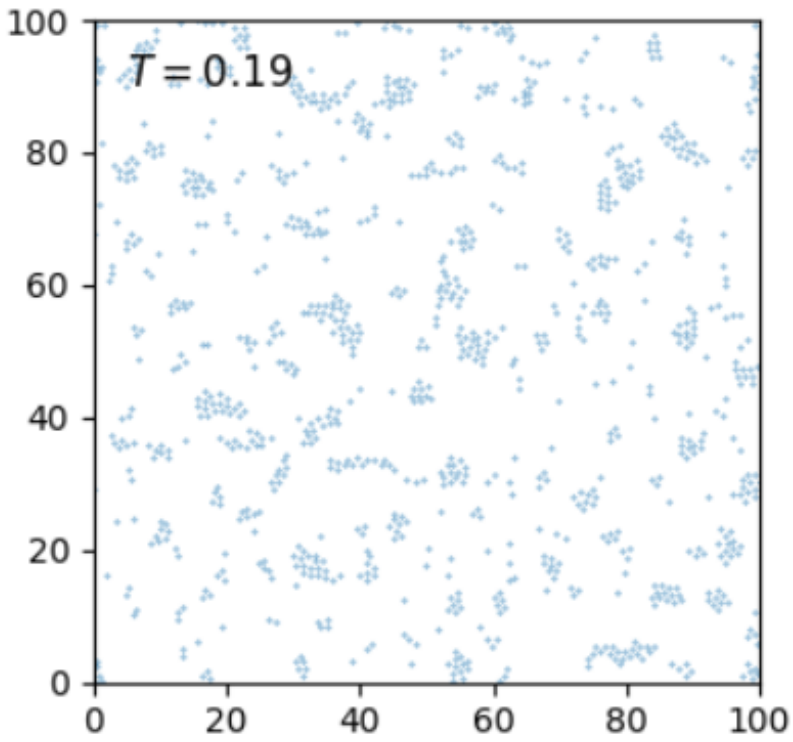

$T = 0.24$
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20

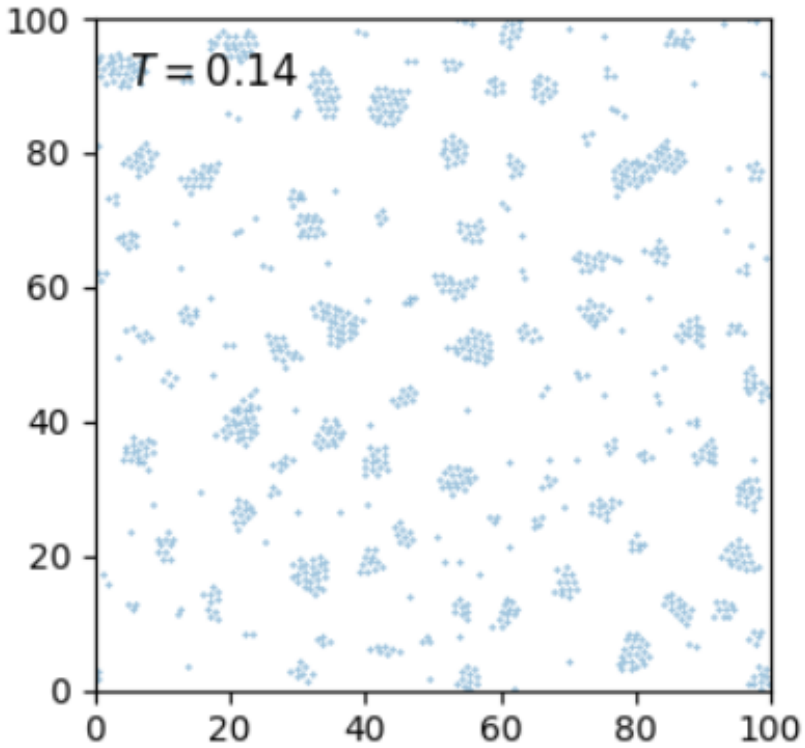

$T = 0.02$
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20

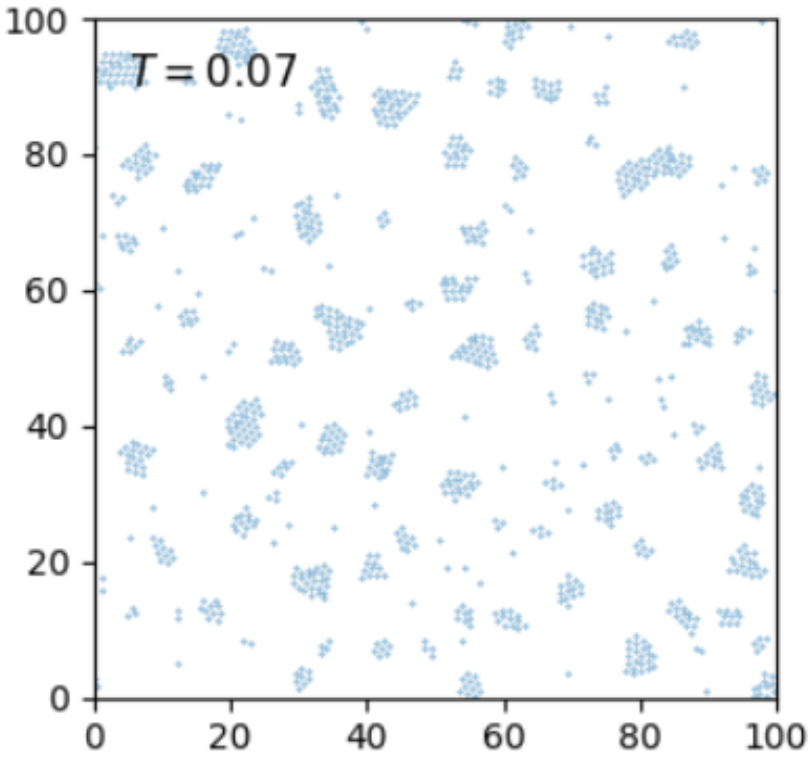
Clustering



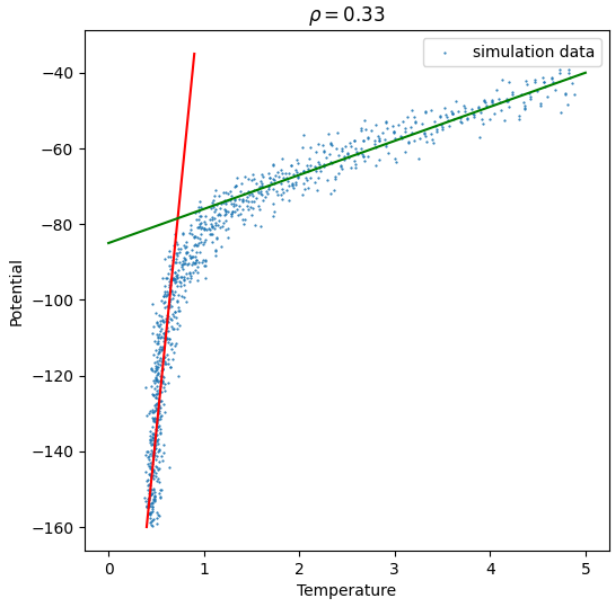

$T = 0.28$
100
80
60
40
20
0
0
20
40
60
80
100


$T = 0.19$
100
80
60
40
20
0
0
20
40
60
80
100


$T = 0.14$
100
80
60
40
20
0
0
20
40
60
80
100


$T = 0.07$
100
80
60
40
20
0
0
20
40
60
80
100

Phase Transition



- Two linear relationships suggest phase change
- Phase changes takes place around $T = 0.6$
- Discontinuous derivatives & nonlinearities

Perspective

- The system is a gas of classical particles interacting via L-J pairwise potential
- Need only know all force-pairs to simulate the system
- Equilibrium states can be simulated so thermodynamic properties can be studied e.g. clustering and phase change