Physics 514 Computational Physics, Fall 2020

Homework 2: Molecular Dynamics

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Author: Yunjie Wang

1 Problem 1

The code for the force looks like the following

```
def force(rsq):
  # Set the constant to 1
  epsilon = 1
  sigma = 1
  sigmasq = sigma ** 2
  r = np.sqrt(rsq)

  return (24*epsilon/r)*((-2)*(sigmasq/rsq)**6+(sigmasq/rsq)**3)
```

2 Problem 2

I set the total time for the integrator to be 60s, and the Δt to be 10^{-3}s. And the forward Euler algorithm "blows up" really fast, while the velocity verlet gives a reasonable result. I just iterate 2s with the same Δt, the result is good enough to see the trend. And also, we could see that the energy for fluid is not that stable even with the Verlet algorithm.

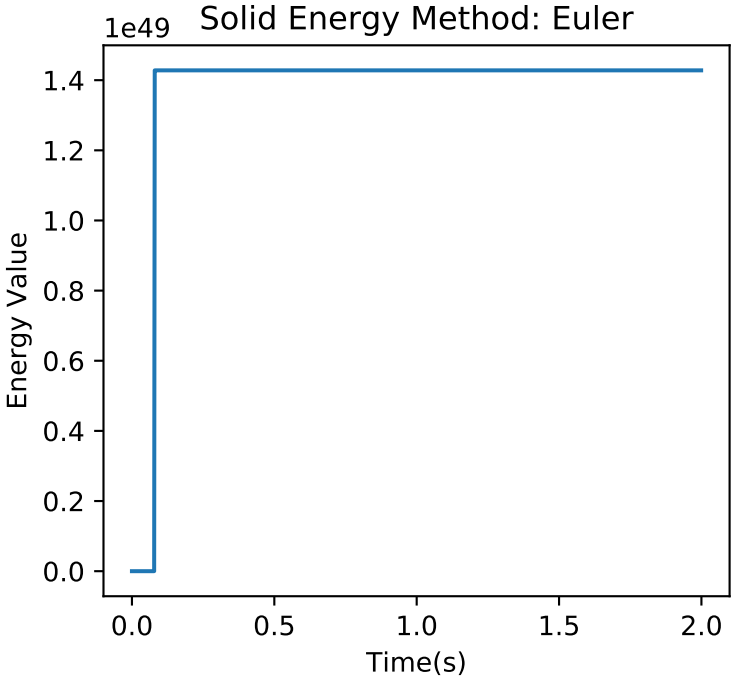
3 Problem 3

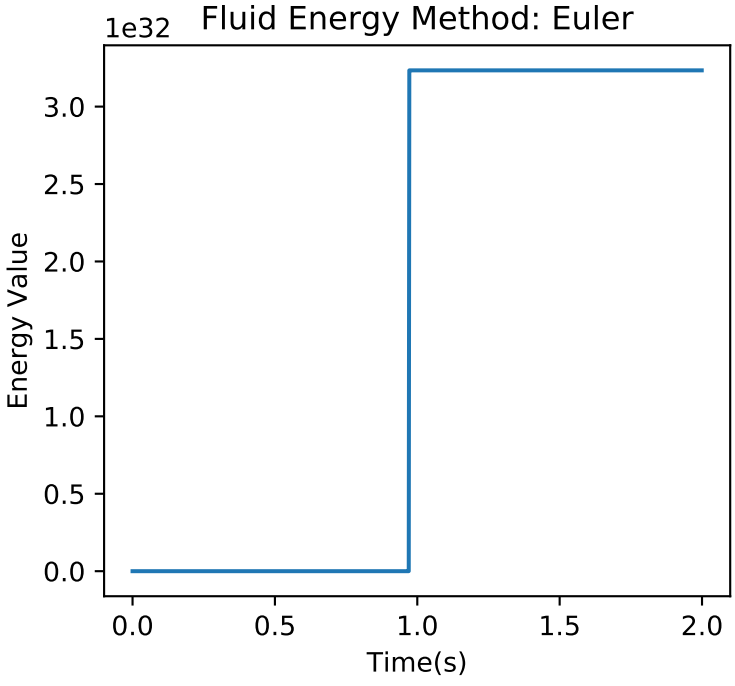
By inspecting several plots, the time to be thermalized for both systems is around 10s. And I include the .mp4 files in the zip folder and please read the README at the beginning of the file.

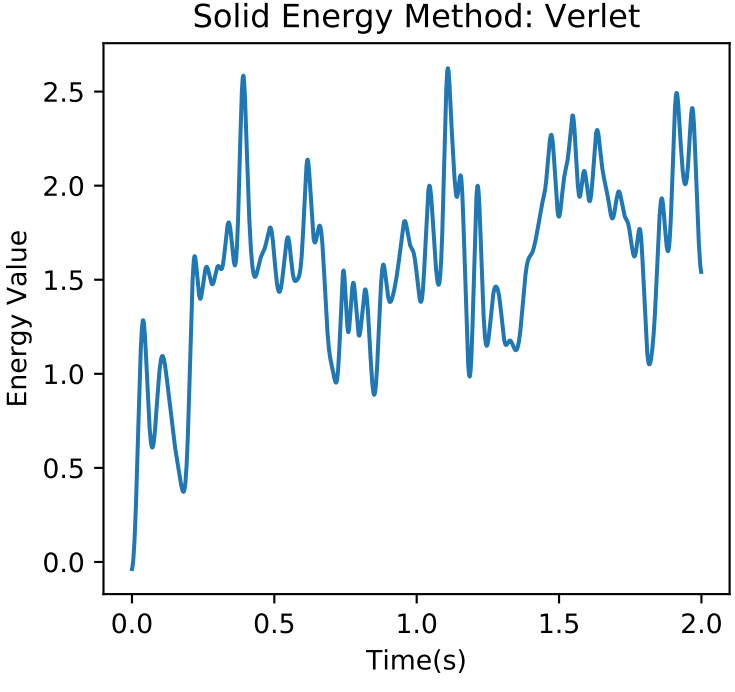
4 Problem 4

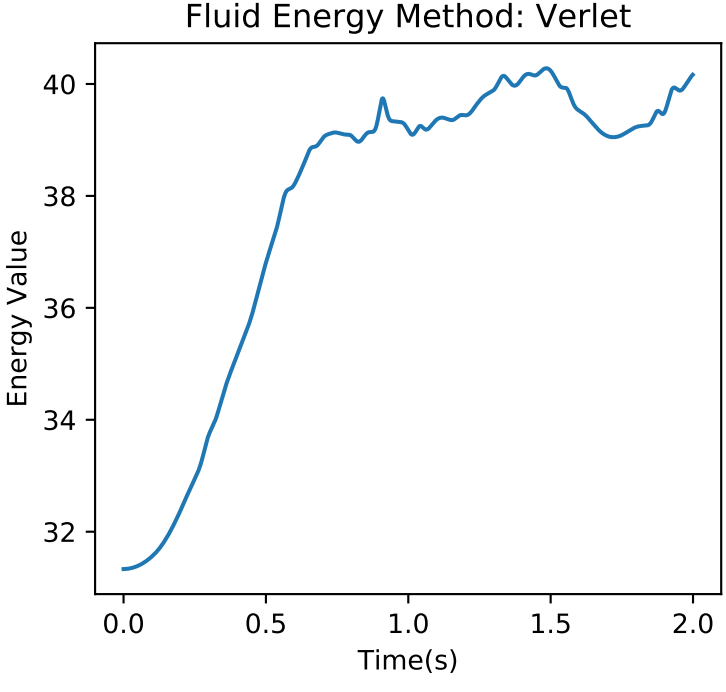
Ref: http://www.physics.emory.edu/faculty/weeks/idl/gofr.html

Energy Visualization

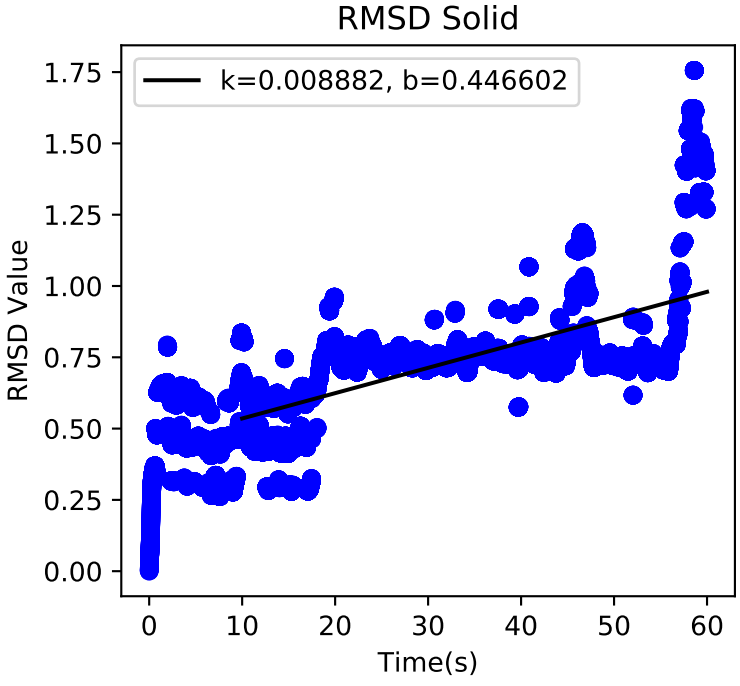


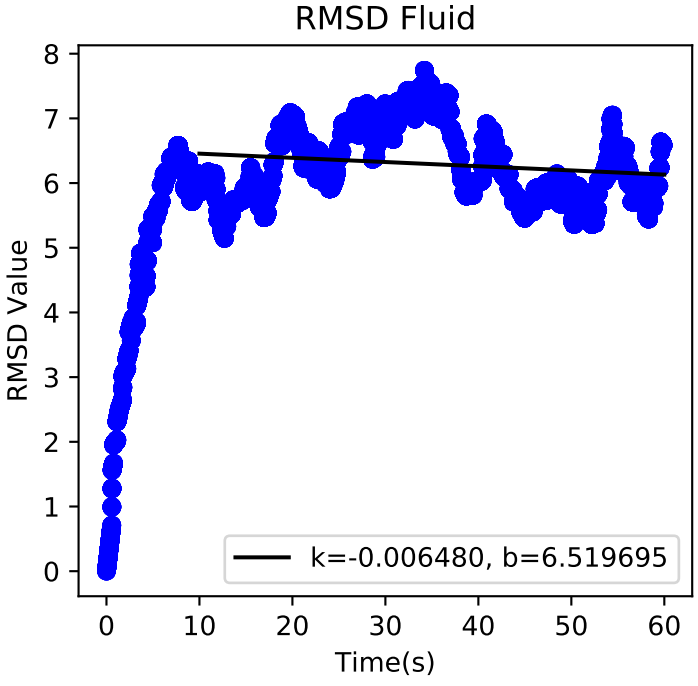


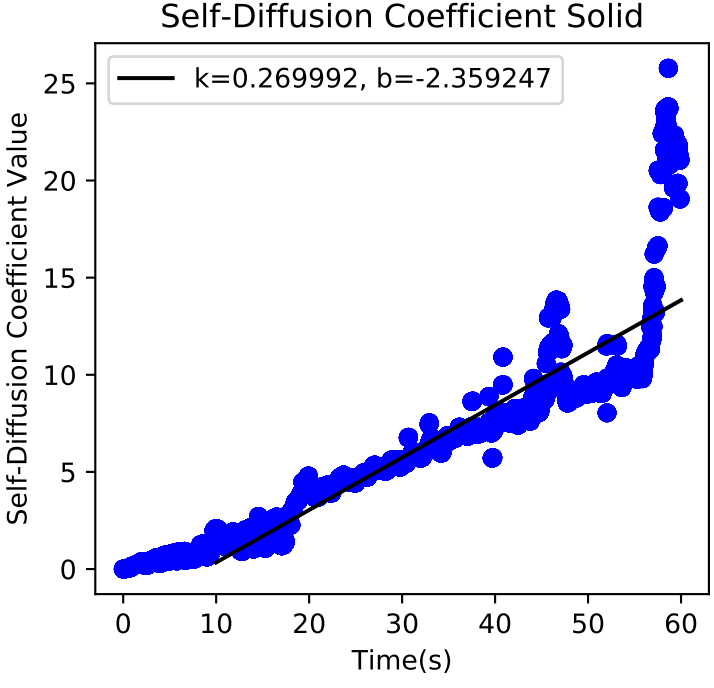


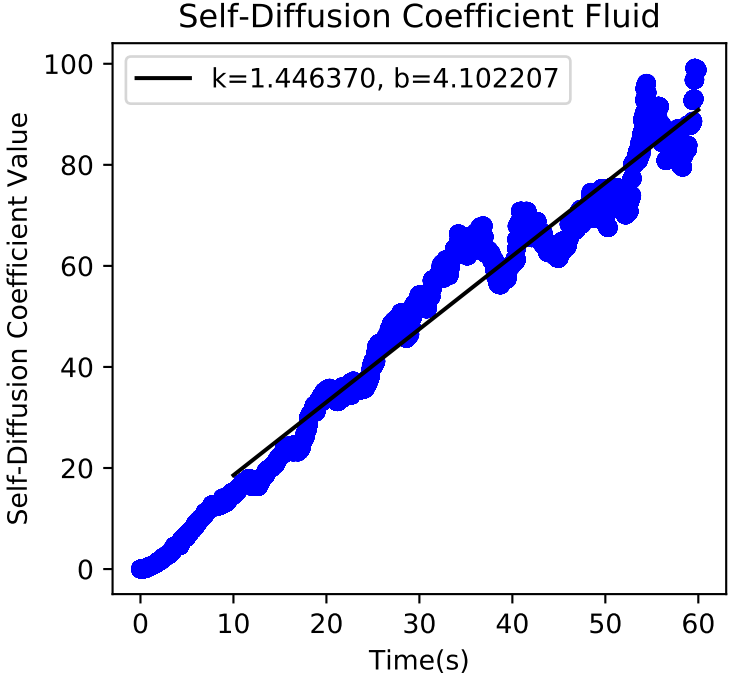


Measurement I









Measurement II