

Report on **Project: Computer simulations of molecular liquids**

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Abstract

In this project, I applied molecular simulation methods to studying the properties of a 2D system of particles. The methods include molecular dynamics (MD) and Metropolis Monte Carlo (MC) simulation. I modeled the system using different model interaction potentials among the particles, including Lennard-Jones (LJ) potential, model atomic potential and model colloidal potential, all pairwise and with a cut-off distance r_c . With carefully chosen initial conditions and boundary conditions, I was able to realize equilibrium states, calculate average total energies and deviations, calculate the radial distributions functions, evaluate the pressure, etc. **Special notes:**

1 Introduction

This is the final project of the course Introduction to Computational Physics. The project is aimed at testing our ability to implement the algorithms we learned in class through programming. The

2 Background

Give a brief summary of the physical theory, include any equations necessary, and cite any references you want to include. Here is how you insert an equation. According to references [?, ?, ?] the dependence of interest is given by

$$\mathcal{L} = \frac{1}{2}m\ell^2(\dot{\theta} + \dot{\phi}_0)^2 - mg_e(t)\ell \cos(\theta)$$

$$m\ell^2(\ddot{\theta} + \ddot{\phi}_0) = mg_e\ell \sin(\theta)$$

$$\ddot{\phi}(t) = -\frac{g_e(t)}{\ell} \sin(\phi(t) - \phi_0(t)) \tag{1}$$

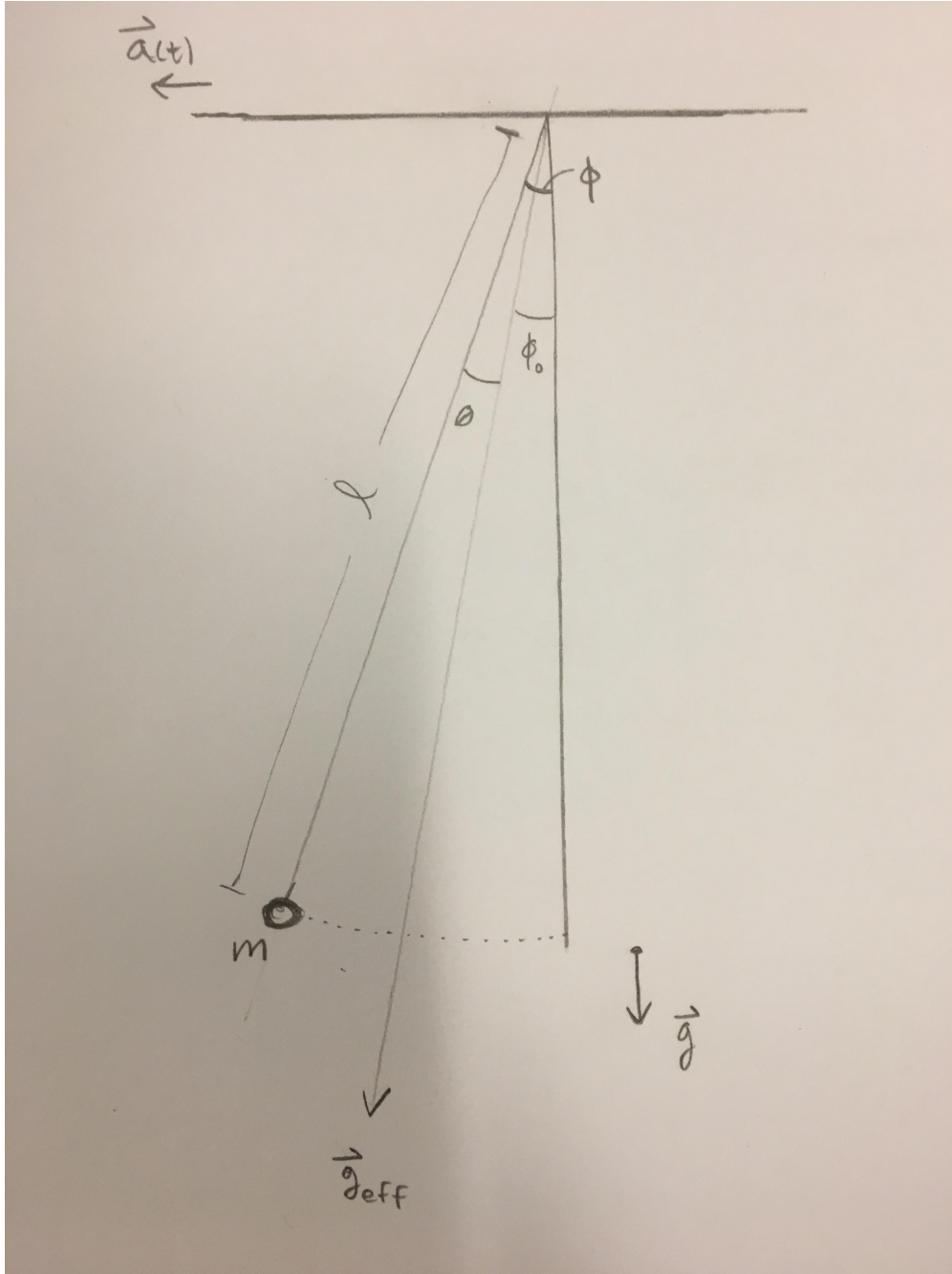


Figure 1: Pendulum that starts at rest in an accelerating frame. If the acceleration is not constant then the apparent vertical, and thus ϕ_0 will change with time

3 Simulations

Give a schematic of the experimental setup(s) used in the experiment (see figure ??). Give the description of abbreviations either in the figure caption or in the text. Write a description of what is going on.

3.1 TASK1

3.2 TASK2

3.3 TASK3

3.4 TASK4

3.5 TASK5

and eventually arrived to the balanced photodiode as seen in the figure ??.

4 Results

In this section you will need to show your experimental results. Use tables and graphs when it is possible. Table 1 is an example.

Table 1: Every table needs a caption.

x (m)	V (V)
0.0044151	0.0030871
0.0021633	0.0021343
0.0003600	0.0018642
0.0023831	0.0013287

Analysis of equation ?? shows ...

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For example, it is easy to conclude that the experiment and theory match each other rather well if you look at Fig. ?? and Fig. ??.

5 Conclusions

Here you briefly summarize your findings. Did you learn any new physics? Was everything as expected?

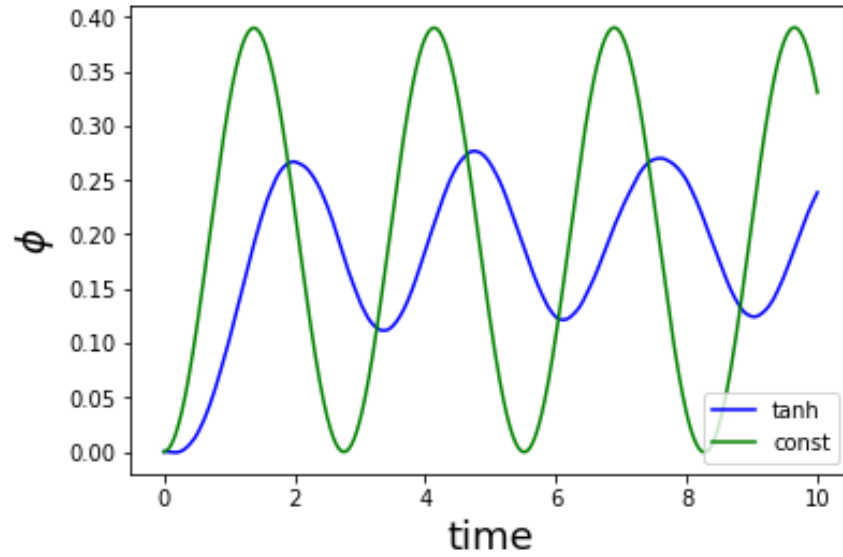


Figure 2: Hyperbolic tangent acceleration vs immediate constant acceleration. The slow approach to the same asymptotic value of 2 meters per second per second induces a lag in the oscillation and also diminishes the amplitude of oscillation.

6 Future Work

Since you had limited time to work on this project, what questions are left outstanding? What would be your next steps?

References