Exam II

5/1/2025

Late 100 Points Possible

Attempt 1

5/1/2025

NEXT UP: Review Feedback

Attempt 1 Score:
N/A

Add Comment

Unlimited Attempts Allowed

5/1/2025

Details

Use the following initial conditions for a triangular lattice of particles:

- N = 64 particles
- Use your modified version of Gould's function **setTriangularLattice** to set positions
- $L_x(0)$ = 9, the horizontal size of the domain at time zero
- $L_y(0)$ = $\frac{\sqrt(3)}{2}L_x$, the vertical size of the domain at time zero
- kT = 1, set from your modified version of the function **setVelcocities** in Gould
- Use dt = 0.005.

While the simulation runs change the size of the box according to the following equations:

$$L_x(t) = A\sin(\frac{2\pi}{\gamma}t) + L_x(0)$$

$$L_y(t) = A\sin(\frac{2\pi}{\gamma}t) + L_y(0)$$

Use amplitude A =1.2 length units, period γ = 2.5 time units, and t=0 at the beginning of the simulation. Be sure to recognize the difference between time in scaled units, t, and the number of time steps that have occurred.

Run the simulation for 8 time units before stopping.

Address each of the following in your write-up:

1. Plots of total energy, temperature, and pressure through the 8 time unit period. Specify the amount of time averaging that has been applied for pressure and temperature plots. Include any other information like heat capacity or raw temperatures that you might have.
2. Plots of the particles at the point of maximum and minimum density. Work out when these occur from the sinusoidal functions.
3. A plot of $\frac{\Delta E}{\Delta T}$ vs time for the entire 8 time unit period. Here ΔE is the change in total energy between two time steps and ΔT is the change in temperature between two time steps.

4. Provide at least one paragraph of commentary and one supporting plot about each of the following sets of questions:
    A. Is energy conserved across a single cycle? Why or why not? Are deviations in energy conservation from the physics of the simulation, or are they the result of numerical approximation?
    B. Is energy conserved between cycles? Why or why not? Are deviations in energy conservation from the physics of the simulation, or are they the result of numerical approximation?
    C. Do phase transitions occur? How do you know? How would you describe them, eg solid to liquid, liquid to gas, etc?
5. Repeat the experiment keeping the temperature as close to constant as possible by calling your version of Gould's **setTemperature** function every time step. Update velocities accordingly. Keep the temperature at kT=1. Address the following questions a second time.
    A. Is energy conserved across a single cycle? Why or why not? Are deviations in energy conservation from the physics of the simulation, or are they the result of numerical approximation?
    B. Is energy conserved between cycles? Why or why not? Are deviations in energy conservation from the physics of the simulation, or are they the result of numerical approximation?
    C. Do phase transitions occur? How do you know?
6. You may have noticed that while the temperature is set to kT=1, it wanders away from that value. Come up with a theory of why that is, state your theory, and test it by modifying something in your code and conducting another run. Add relevant support for your theory/test in the form of output plots and commentary.

Notes:

1. This simulation works fine on my code base and requires less than five seconds without graphics. For the sake of efficiently completing the exam, I strongly recommend doing as much work as you can *without* graphics.
2. If you are having difficulty because of numerical instability, begin by looking at what is happening over a single cycle, hopefully that can work and reporting on it should get you as many of the points available. If that works try and make A and/or dt smaller, that can help too. Emphasize getting something done for each of the above prompts, even if the simulation is much simpler. Some important observations come from comparing at least two successive cycles, so work hard to get at least that. Three cycles shows more of the same.
3. You may use the heat capacity determined from fluctuation (book's formula) if you have it implemented. It could provide interesting discussion points. However, it is not required.
4. You may use the same plot to satisfy the requirements, and to structure commentary around. Consider annotating the plots to call the reader's attention to certain features. Don't be too fancy - just use simple software to draw on top of your images.
5. An especially useful annotation on plots is the time when the maximum and minimum domain sizes occur. Try to add this.

6. Don't worry too much if your output gives more than the required information, just use that and I'll find/figure out what you're talking about. Annotate your plots to help me find it.

Submission

- I do not think that using a Jupyer notebook is necessarily the best way to finish this. Instead, if you can, run a script, get a plot, and paste it into a document. That said, if you're set up to go with Jupyter, go! Please save and upload your submission ***as a PDF file.***
- Maintain the numbering scheme above in your report to make it easier for me to figure out what you are responding to.
- To open the door to partial credit, include all source code as part of your submission.

	File Name	Size	
	LJVisualizer.py	5.04 KB	
	LJSimulator.py	11.8 KB	
	Exam 2.html	8.07 MB	
	Exam 2.pdf	1.28 MB	