

Lab exploration 3: Particle systems

Math 309 Fall 2019

Deadline: class 7 October

- Conduct experiments as directed.
- **Journal entry.** Respond to each of the “journal queries.” Using *concise and clear sentences*, incorporate data, symbols, and illustrations into your text. Have an audience in mind. Focus on *developing* an explanation or argument that stems from your simulations.
Submit 300-400 words double-spaced in **hard copy**.
- **Recommended.** Work in groups of 2 or 3. Submit one journal entry for the group.

Models are located in the [Models Library](#) under the heading [GasLab](#). Before running the simulations, read the “What is it?” and “How it works” sections under the [Info](#) tab.

Model: GasLab Adiabatic Piston. Configure the simulation with the following settings (leave omitted parameters at the default settings).

```
number-of-particles = 200
init-particle-speed = 5
particle-mass = 1
piston-mass = 2000
```

Run the process for around 300 time steps (ticks). There’s a slider that controls the speed.

3.1 Journal query.

Watch the [Piston Height](#) and [Pressure](#) graphs and note the resulting oscillating behavior. How long—in time steps—does it take the process to go through one cycle? Briefly explain the appearance of the oscillations. Also, notice and describe the difference between the form of the pressure-time graph at the peaks and troughs. Explanation?

3.2 Journal query.

Experiment with various settings of the parameters in an attempt to produce non-oscillating behavior. Which settings are crucial for this outcome? Why?

Model: GasLab Two Gas. Begin with the settings below.

```
collide? - on
box-size = 100%
opening-size = 20%
num-magentas = 10
num-cyans = 10
magenta-init-speed = 50
cyan-init-speed = 50
magenta-mass = 5
cyan-mass = 5
```

3.3 Journal query.

What do you expect the long-term tendency in the behavior of the system to be? Why should we think of this state as an equilibrium? Allow the simulation to run until the system gets close to that state—say, within 10% of equilibrium. How many time steps does it take to reach near-equilibrium?

Let the system go until it's near equilibrium. If the system continues to run, does the macrostate—number of particles of each type on either side of the chamber—depart from being within 10% of equilibrium?

Recall that the entropy of a macrostate is given by the number of microstates—location of each particle relative to a side of the chamber—that produce the given macrostate. What happens to the entropy as the system evolves? Is there a maximum entropy macrostate? If so, what is it?

3.4 Journal query.

Change only the settings

```
num-magentas = 100
num-cyans = 100.
```

What's the equilibrium state now? How many time steps does it take to get within 10% of equilibrium? If you get a significantly different result than in the previous case, what accounts for the difference?

Let the system go until it's near equilibrium. If it continues to run, does the macrostate depart from being within 10% of equilibrium? Compare to the previous case with 10 particles of each type.

3.5 Journal query.

With 500 particles of each kind, set

```
opening-size = 99%
magenta-init-speed = 50
cyan-init-speed = 5
```

and leave the remaining parameters the same. Describe the initial macrostate of the system in terms of temperature. What's the system's equilibrium macrostate? What does the evolution of the system tell us about heat transfer?

Model: GasLab Maxwells Demon. This model simulates a thought experiment proposed by J. C. Maxwell. In a two-gas system with a divider and a window operated by a demon, particles on the left side that approach the window with a speed above a certain threshold value are allowed to pass to the right side while particles on the right that approach the window with a speed below the threshold are allowed to pass to the left side.

3.6 Journal query.

Select values for the settings that could be considered to produce an equilibrium. What's the initial macro-state in terms of temperature? Run the model and describe how the macro-state evolves. Compare this process to that of the two-gas model executed previously. A natural macrostate here is how many particles of each type (slow/fast) are there on either side of the chamber. What's happened to the system's entropy? That is, how do the macrostates evolve in time? Do you see why the demon-modulated process seems to violate the second law of thermodynamics?