

## Lab 7

### Learning Objectives:

- I. **What characters do I type next?** *What are the most important functional elements of classes and objects in Python?* This lab will give you the opportunity to learn the major syntax and functionality associated with classes in Python.
- II. **How do I plan a project and execute my plan?** *How do I organize and write object-oriented code?* This class will give you the opportunity to practice organizing code around classes and objects.
- F. **Write and Test, Write and Test....** *Write code in small bits that you can easily test.* If you code an enormous project and then test it all at once, how do you know where your error is? This lab gives you the opportunity to practice testing your code at regular intervals. Object-oriented programming makes it particularly easy to organize code in ways that can be tested.

### Part I: Writing Classes for a Diatomic Molecule

Today's lab guides you through creating a simulation of the motion of a diatomic molecule. In this part, **your task is to create a Molecule class that to store and calculate information about diatomic molecules.**

For this part of the lab you will be writing code to simulate two particles connected together by a compressible bond. You will be creating and using a **Molecule** class that contains information about the entire two-particle system as well as a **Particle** class which contains basic information about each subparticle.

Begin by examining the already implemented **Particle** class in **particle.py**. See what data is stored in each **Particle** object and how you would access it. Try creating a particle by calling the constructor. Then try modifying its attributes and confirm that they changed.

You need to create a **Molecule** class that contains the following attributes and methods:

- Two attributes **p1** and **p2** that are Particle objects (representing the two subparticles);
- An attribute **k**, the spring constant of the bond connecting the two subparticles;
- An attribute **L0**, the equilibrium length of the bond
- A constructor that accepts the following:
  - The initial positions of the two particles
  - The masses of the two particles
  - The spring constant and equilibrium length of the molecule
- A method **get\_displ** that returns the vector pointing from the location of particle **p1** to the location of particle **p2**. This should be a one-liner.
- A method **get\_force** that returns the force (vector) due to the spring on particle **p1**.

Implement this class and make sure that your **get\_force** function it is working before continuing onward!

## Part 2: Using Your Molecule Class for Calculating Dynamics

Now that you've written the Molecule class, **your task is to use it to simulate the motion of a diatomic molecule.**

We have provided you the file `dynamics.py`, which is set up to animate the movement of the particle. You will need to do a few things within this file:

- In `init_molecule`, create and return an instance of your `Molecule` class. The initial position should satisfy  $x_0, y_0 \in [0, 1]$ .
- In `time_step`, update the positions of the two particles in molecule `mol` after a time `dt`. **There's no need to return anything; the starter code can look inside the object when animating!** We suggest you use the following algorithm for updating (called *leapfrog integration*).
  - (Optional) **Background on leapfrog integration:** Newton's Second Law is a 2nd-order ODE, so we can split it up into two coupled first order ODEs:  $\frac{dv}{dt} = a = F(x)/m$  and  $\frac{dx}{dt} = v$ . Approximately, then (i.e. using Euler's method),  $\Delta v = (F(x)/m)\Delta t$  and  $\Delta x = v\Delta t$ . Since these finite differences are most accurate about halfway between the endpoints used to calculate them, we'll calculate  $x$  and  $a$  at integer multiples of  $\Delta t$  and  $v$  at half-integer multiples of  $\Delta t$ .
  - (Optional) **The algorithm, in depth:**
    - i. Start with  $i = 0$ .
    - ii. Increment  $t_i$  by  $\Delta t/2$  to give  $t_{i+1/2}$ .
      - Calculate  $v(t_{i+1/2}) = v(t_{i-1/2}) + (F(x(t_i))/m)\Delta t$ . (Let  $v(t_{-1/2})$  indicate the initial velocity.)
    - iii. Increment  $t_{i+1/2}$  by  $\Delta t/2$  to give  $t_{i+1}$ .
      - Calculate  $x(t_i) = x(t_i) + v(t_{i+1/2})\Delta t$ .
    - iv. Increase  $i$  by 1 and repeat steps ii. through iv.
  - **As long as there's no explicit time dependence, this is pretty much as simple as alternately updating  $x$  and  $v$ .** Your job is to implement this using the objects you've created!

Of course you'll want to test your code. Try using

- starting positions (0.2, 0.2) and (0.8, 0.8);
- masses 1 and 2;
- spring constant  $k = 1$ ; and
- equilibrium length  $L_0 = 0.5$ .

Things to look for: Does the molecule behave like a spring? Does the heavier particle move less than the lighter particle?

## Part 3: If You Have Time, Implement Initial Velocity

If the initial angular momentum of your molecule is zero, it will spin! **Figure out how to set nonzero initial**

**velocities for your particles, and then run the simulation again.**