*** Names: Ryogo, Bibi ***

Lab 5: N-body simulations

In this lab, adapted from Philip Mocz's public repository, you will write your own simple N-body simulation code! Then we'll compare it to the code REBOUND, a popular N-body code used for astrophysics research.

```
# As usual, import some useful packages
import numpy as np
import matplotlib.pyplot as plt
```

Day 1: Writing our own N-body code

Part 1: Some useful functions

Recall that the first step of any N-body code is to calculate the *acceleration* of each particle, caused by its gravitational interactions with all the other particles. To make this easier, let's write a function to calculate an *array* of accelerations.

In the following code, make sure to respond to all `TODO` s!

```
def getAcc( pos, mass, G, softening ):
  """
    Calculate the acceleration on each particle due to Newton's Law
  Inputs:
      pos (array): N x 3 matrix of positions
      mass (array): N x 1 vector of masses
      G (float): Newton's gravitational constant
      softening (float): softening length
  Outputs:
      a (array): N x 3 matrix of accelerations
  """

  # Get positions r = [x,y,z] for all particles
  x = pos[:,0:1]
  y = pos[:,1:2]
  z = pos[:,2:3]

  # Store all pairwise particle separations: r_j - r_i
  dx = x.T - x
  dy = y.T - y
  dz = z.T - z

  # Compute the magnitude of all particle pairwise particle separations
  # TODO: fill in the definition of r^2 (use dx, dy, and dz)
  r_sq = dx**2+dy**2+dz**2
  r_sq += softening**2
  r = r_sq
  r[r>0] = r[r>0]**(-1.5)

    # Calculate x, y, and z components of acceleration
  # TODO: What does the @ symbol here mean? Use whatever resources you need to figure it out, and comment your answer below.
  # Answer: Matrix multiplication.
  ax = G * (dx * r) @ mass
  ay = G * (dy * r) @ mass
  az = G * (dz * r) @ mass

  # Pack together the acceleration components
  a = np.hstack((ax,ay,az))

  return a
```

Let's also write a function to calculate the kinetic and potential energy of the system.

```
def getEnergy( pos, vel, mass, G ):
    """
    Get kinetic energy (KE) and potential energy (PE) of simulation
    Inputs:
        pos (array): N x 3 matrix of positions
        vel (array): N x 3 matrix of velocities
        mass (array): N x 1 vector of masses
        G (float): Newton's gravitational constant
    Outputs:
        KE (float): kinetic energy of the system
        PE (float): potential energy of the system
    """

    # TODO: fill in the kinetic energy here (hint: you will need to use multiple np.sum() commands!)
    KE = 0.5 * np.sum(np.sum(mass * vel**2))

    # Now let's compute potential energy!
    # TODO: Based on the code in the previous function, compute dx, dy, and dz

    # Get positions r = [x,y,z] for all particles
    x = pos[:,0:1]
    y = pos[:,1:2]
    z = pos[:,2:3]

    # Store all pairwise particle separations: r_j - r_i
    dx = x.T - x
    dy = y.T - y
    dz = z.T - z

    # Compute the inverse magnitude of all pairwise particle separations 1/r
    inv_r = np.sqrt(dx**2 + dy**2 + dz**2)
    inv_r[inv_r>0] = 1.0/inv_r[inv_r>0]

    # Sum over upper triangle (to count each interaction only once)
    PE = G * np.sum(np.sum(np.triu(-(mass*mass.T)*inv_r,1)))

    return KE, PE
```

Questions

1. The `getAcc()` function has a parameter called the "softening length." What is this parameter? Skim the introduction of this paper (Zhang et al. 2019), and write a 1-2 sentence explanation of what the softening length is and why it's important.

> Answer: The softening length is a measure of the volume of a particle. This is important because our particles are not point masses, so close interactions will behave differently.

2. Look at the line in `getEnergy()` starting with `PE = ...`. What is the equation being used to compute potential energy?

> Answer: $U = \Sigma \frac{Gm_i m_j}{r_{ij}}$

Before you move on to the next part, ask Prof Mia to look over your code to make sure it'll run!

Part 2: Run the N-body simulation

Now let's set up and run the actual simulation! As always, make sure to respond to all `TODO` comments below.

```
def runSimulation(N, dt, tEnd=10.0, softening=0.1, G=1.0, plotRealTime=True):
    """ Run simple N-body simulation of random particles
    Inputs:
        N (int): number of particles
        dt (float): timestep size
    Keywords:
        tEnd (float): time at which simulation ends
        softening (float): softening length
        G (float): Newton's gravitational constant
        plotRealTime (bool): if True, plot as the simulation runs
    """
    # Initial conditions
    t = 0                         # initial time
    Nt = int(np.ceil(tEnd/dt))  # number of timesteps
    np.random.seed(17)            # set the random number generator seed
    mass = 20.0*np.ones((N,1))/N  # total mass of particles is 20
    pos  = np.random.randn(N,3)   # randomly selected positions
    vel  = np.random.randn(N,3)   # randomly selected velocities

    vel -= np.mean(mass * vel,0) / np.mean(mass)  # convert initial velocities to Center-of-Mass frame
    acc = getAcc( pos, mass, G, softening )  # calculate initial gravitational accelerations
    KE, PE  = getEnergy( pos, vel, mass, G )  # calculate initial energy of system

    # Set up some empty arrays to store variables (these will be useful for making plots!) and put in initial values
    pos_save = np.zeros((N,3,Nt+1))
    pos_save[:,:,0] = pos
    vel_save = np.zeros((N,3,Nt+1))
    vel_save[:,:,0] = vel
    KE_save = np.zeros(Nt+1)
    KE_save[0] = KE
    PE_save = np.zeros(Nt+1)
    PE_save[0] = PE
    t_all = np.arange(Nt+1)*dt

    # Prep figure
    if plotRealTime:
        %matplotlib qt
        fig = plt.figure(figsize=(4,5), dpi=80)
        ax1 = plt.subplot()

    # This is the main loop of the simulation!
    for i in range(Nt):

        # calculate accelerations
        acc = getAcc( pos, mass, G, softening )

        # TODO: update velocities (using the acceleration you just calculated)
        vel = vel + acc * dt

        # TODO: update positions (using the updated velocity you just calculated)
        pos = pos + vel * dt

        # TODO: update time
        # t += dt
        # t_all[i+1] = t

        # TODO: get energy of system
        KE, PE  = getEnergy( pos, vel, mass, G )

        # save energies, positions for plotting trail
        pos_save[:,:,i+1] = pos
        vel_save[:,:,i+1] = vel
        KE_save[i+1] = KE
        PE_save[i+1] = PE

        # plot in real time
        if plotRealTime:
            plt.sca(ax1)
            plt.cla()
            xx = pos_save[:,0,max(i-50,0):i+1]
            yy = pos_save[:,1,max(i-50,0):i+1]
            plt.scatter(xx,yy,s=1,color=[.7,.7,1])
            plt.scatter(pos[:,0],pos[:,1],s=10,color='blue')
            ax1.set(xlim=(-2, 2), ylim=(-2, 2))
            ax1.set_aspect('equal', 'box')
            ax1.set_xticks([-2,-1,0,1,2])
            ax1.set_yticks([-2,-1,0,1,2])

            plt.pause(0.001)

    # Save figure
    if plotRealTime:
        plt.close()

    return KE_save, PE_save, t_all
```

```
# First simulation run!
KE_save, PE_save, t_all = runSimulation(N=100, dt=0.01)
```

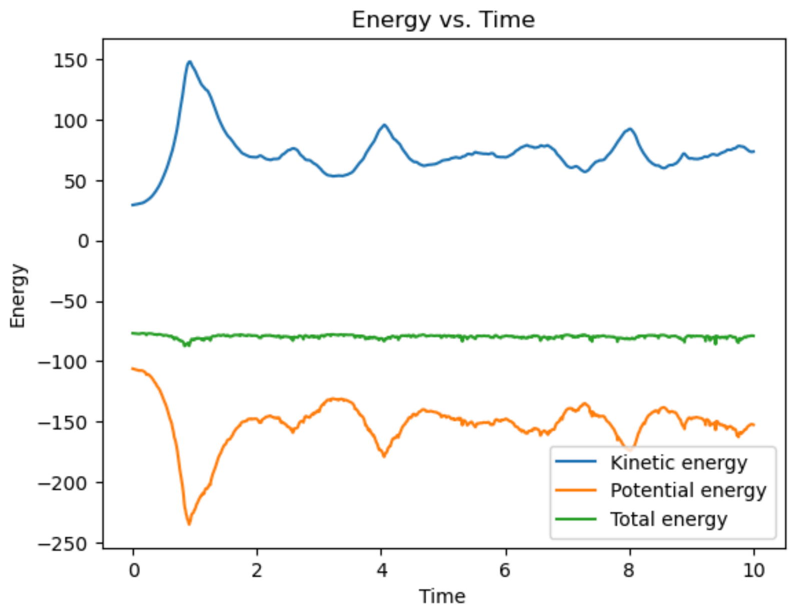
```
# For the following questions, make sure plots are inline
%matplotlib inline
```

Questions

1. Make a plot of the kinetic energy, potential energy, and total energy (KE+PE) of the system as a function of time. Make sure your axes are labeled appropriately, and use different line colors/styles to represent each line (which should be labeled in a legend!).

```
# Code for question 1
plt.plot(t_all, KE_save, label='Kinetic energy')
plt.plot(t_all, PE_save, label='Potential energy')
plt.plot(t_all, PE_save+KE_save, label='Total energy')
plt.legend()
plt.xlabel('Time')
plt.ylabel('Energy')
plt.title('Energy vs. Time')
```

```
Text(0.5, 1.0, 'Energy vs. Time')
```



Questions (cont.)

2. What is the approximate relationship between the kinetic energy and potential energy? Does this make sense, given what we know about systems in quasi-equilibrium?

> Answer: It is the negative of the potential energy minus a constant (between 50 and 100). Yes, this makes sense because in systems in quasi-equilibrium, energy is conserved.

3. Why is the total energy negative?

> Answer: The system is gravitationally bound.

Day 2: REBOUND

You may have noticed in the previous plot that the total energy is not quite constant in our simulation. Let's quantify this!

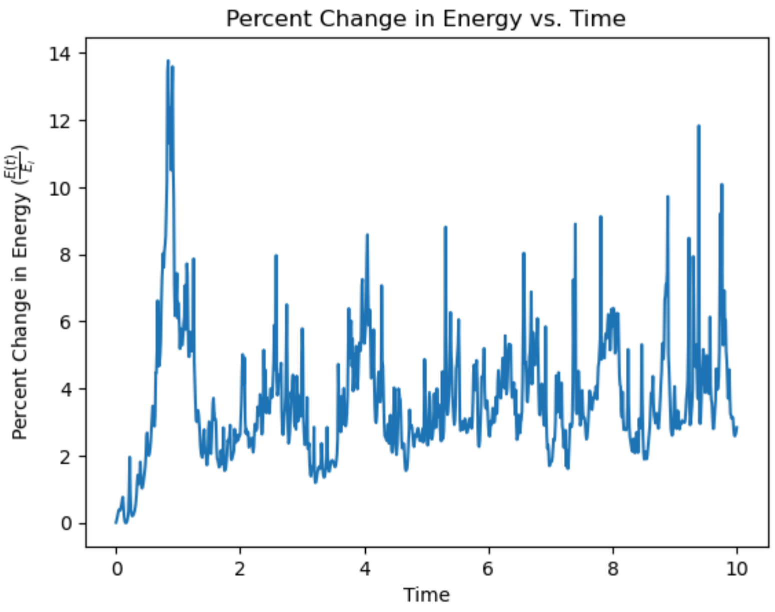
Part 1: Conservation of energy?

Questions

1. Plot the percent change in total energy as a function of time. At the end of the simulation, by what percent has the total energy of the system changed? The total energy changed by about 2 percent.

```
# Code for question 1
TE = PE_save+KE_save
plt.plot(t_all, 100*TE/TE[0] - 100)
plt.xlabel('Time')
plt.ylabel(r'Percent Change in Energy ($\frac{E(t)}{E_i}$)')
plt.title('Percent Change in Energy vs. Time')
```

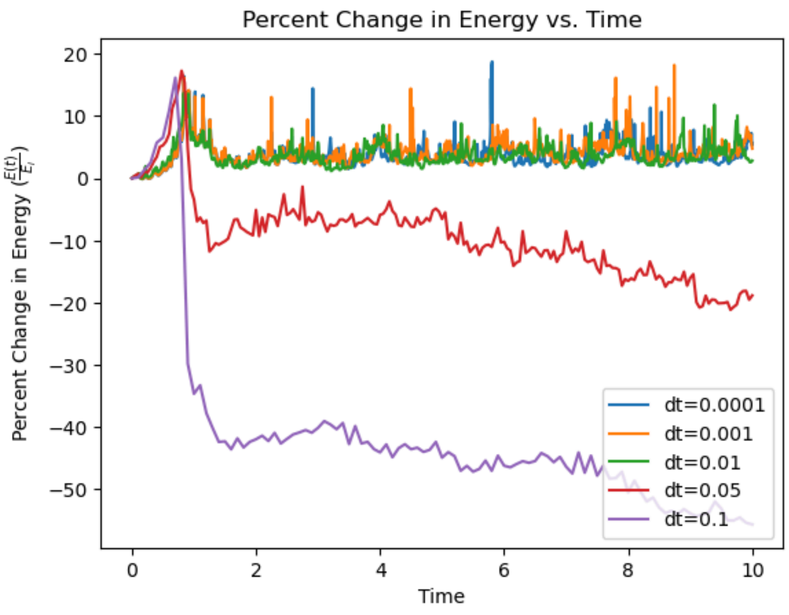
```
Text(0.5, 1.0, 'Percent Change in Energy vs. Time')
```



2. How does the plot above change if you change the size of the timestep `dt`? Run the simulation a few times using different values of `dt` (set `plotRealTime=False` to make this faster, otherwise it might take an unreasonably long time to run!), then plot the percent change in energy as a function of time for each of these runs (i.e., make a version of the above plot with different lines showing the results for different values of `dt`). Make sure each line is distinct and labeled (with an attached legend)!

```
# Code for question 2
for dt in [0.0001, 0.001, 0.01, 0.05, 0.1]:
    KE_save, PE_save, t_all = runSimulation(N=100, dt=dt, plotRealTime=False)
    TE = PE_save+KE_save
    plt.plot(t_all, 100*TE/TE[0] - 100, label=f'dt={dt}')
plt.xlabel('Time')
plt.ylabel(r'Percent Change in Energy ($\frac{E(t)}{E_i}$)')
plt.title('Percent Change in Energy vs. Time')
plt.legend(loc='lower right')
```

```
<matplotlib.legend.Legend at 0x177d01890>
```



Part 2: REBOUND

Now let's try comparing our results against a research-grade N-body code called **REBOUND**.

```
%pip install rebound
```

```
Defaulting to user installation because normal site-packages is not writeable
Requirement already satisfied: rebound in /Users/bhanselman27/.local/lib/python3.11/site-packages (4.4.7)
Note: you may need to restart the kernel to use updated packages.
```

```
import rebound
```

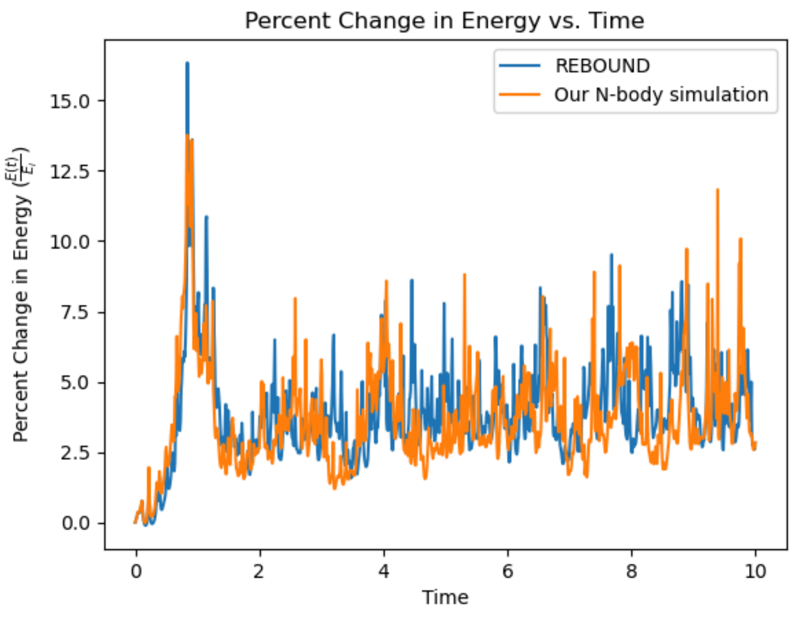
```
# You don't need to modify anything in this cell

def runRebound(N, dt, tEnd=10.0, softening=0.1, G=1.0, plotRealTime=True):
    """ Set up REBOUND N-body simulation of random particles
    Inputs:
        N (int): number of particles
        dt (float): timestep size
    Outputs:
        times (array): array of timesteps
        energy (array): array of total energy
    Keywords:
        tEnd (float): time at which simulation ends
        softening (float): softening length
        G (float): Newton's gravitational constant
        plotRealTime (bool): if True, plot as the simulation runs
    """

    sim = rebound.Simulation()

    # Set the simulation parameters to be the same as our earlier code
    N          = N     # number of particles
    sim.softening = softening    # softening length
    sim.G          = G     # Newton's Gravitational Constant

    # Use the same random number generator seed, so the particles will start in the same place
    np.random.seed(17)             # set the random number generator seed
    mass = 20.0*np.ones((N,1))/N  # total mass of particles is 20
    pos  = np.random.randn(N,3)   # randomly selected positions and velocities
    vel  = np.random.randn(N,3)

    # Add particles to simulation
    for i in range(N):
        sim.add(m=mass[i],x=pos[i,0],y=pos[i,1],z=pos[i,2],vx=vel[i,0],vy=vel[i,1],vz=vel[i,2])
    sim.move_to_com()  # move particles to center of mass frame

    if plotRealTime:
        sim.widget(size=(400,400))

    # Step the simulation forward, and save the energy of the system at each timestep
    times = np.arange(0, tEnd, dt)
    energy = np.zeros(len(times))
    for i, time in enumerate(times):
        sim.integrate(time, exact_finish_time=1)
        energy[i] = sim.energy()

    return times, energy


# First simulation run!
times, energy = runRebound(N=100, dt=0.01,plotRealTime=False)
```

Questions

1. Plot the percent change in total energy as a function of time for both our old N-body code and the REBOUND code. Use `N=100` and `dt=0.01` for both simulations (also recall that setting `plotRealTime=False` will make both `runSimulation()` and `runRebound()` run faster). As always, make sure to use different line colors/styles, labeling the different lines with an appropriate label. Is one of the methods clearly better than the other?

```
# Code for question 1
KE_save, PE_save, t_all = runSimulation(N=100, dt=0.01, plotRealTime=False)
TE_old=KE_save+PE_save
plt.plot(times, 100*energy/energy[0]-100, label='REBOUND')
plt.plot(t_all, 100*TE_old/TE_old[0]-100, label='Our N-body simulation')
plt.xlabel('Time')
plt.ylabel(r'Percent Change in Energy ($\frac{E(t)}{E_i}$)')
plt.title('Percent Change in Energy vs. Time')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x177b9acd0>
```



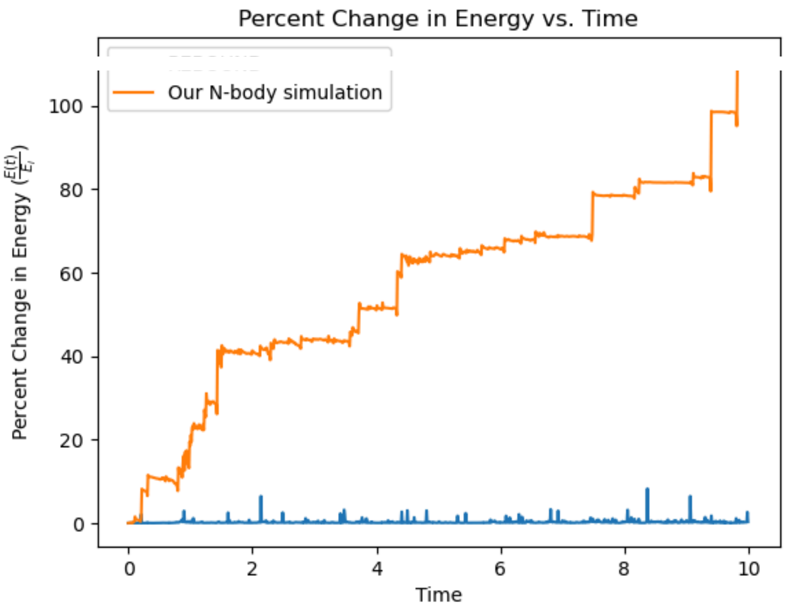
> Answer for question 1: The percent change over time is about the same for both simulations.

2. Do the same thing, but this time set the `softening` parameter to 0.01 (instead of the default 0.1). Now what happens? Why do you think this plot is different from the plot from question 1?

```
# Code for question 2
times, energy = runRebound(N=100, dt=0.01, softening = 0.01, plotRealTime=False)
KE_save, PE_save, t_all = runSimulation(N=100, dt=0.01, softening = 0.01, plotRealTime=False
TE_old = KE_save + PE_save
```

```
plt.plot(times, 100*energy/energy[0]-100, label='REBOUND')
plt.plot(t_all, 100*abs(TE_old/TE_old[0]-1), label='Our N-body simulation')
plt.xlabel('Time')
plt.ylabel(r'Percent Change in Energy ($\frac{E(t)}{E_i}$)')
plt.title('Percent Change in Energy vs. Time')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x31226fd90>
```



> Answer for question 2: Our N-body simulation accrues much more error in the total energy over time while the REBOUND simulation total energy still remains roughly constant. We think this is because the softening parameter added to the radius squared in our simulation lowered the energy changes that resulted from the approximate nature of each integration. When the softening is small, the denominator of the forces approaches the pairwise distance squared, so the errors in the numerical solution at each timestep become much more significant (the forces become larger).

3. The way N-body simulations work is by integrating the equations of motion for each particle (that's what we did when we "updated" the particle velocities and accelerations at each timestep). Our N-body code does this integration using a version of the "semi-implicit Euler method." What integrator does REBOUND use? Look up the REBOUND documentation to find the answer. (Hint: REBOUND can be made to use one of many integrators, but it uses one particular method as its default.) In what 2 main ways is this method different from the semi-implicit Euler method?

> Answer for question 3: REBOUND uses the IAS15 integrator. It uses adaptive timesteps to obtain the most accurate solutions. It also is higher order (Euler is first order, while IAS15 in 15th order).

Submitting Pre-labs and Labs for Grading

Before submitting any notebook for grading, please follow the following steps:

1) Make sure the names of all group members are in a markdown cell at the top of the file.

2) Save the notebook as a PDF. Depending on what program you use, you may need to use some variation of the following command: "File -> Print -> Save to PDF"

3) Upload the PDF to Gradescope. **Make sure all group members' names are on the Gradescope submission, and that all code outputs (and anything you changed in the code, including comments) are visible.**