PS12_Joey_Shin

May 3, 2025

1 Question 1

1.1 (i)

1.1.1 See Code

[2]:
```
# import packages for basic math, plotting, linear algebra, etc.
from numpy import *
from numpy.linalg import *
from numpy.random import *
from matplotlib.pyplot import *
from scipy.special import binom, erf, erfc

class histogram(): # histogram class
    def __init__(self,limits,binwidth):
        self.limits = limits
        self.binwidth = binwidth
        self.vals = arange(self.limits[0] + self.binwidth / 2, self.limits[1],␣
 ↪self.binwidth)
        self.histo = 0 * self.vals
        self.N_samples = 0

    def add_sample(self,dat):
        self.N_samples += 1
        if dat > self.limits[0] and dat < self.limits[1]:
            bin_index = int((dat - self.limits[0]) / self.binwidth)
            self.histo[bin_index] += 1

    def normalize(self):
        self.histo = self.histo / (self.N_samples * self.binwidth)

    def barplot(self):
        bar(self.vals, self.histo, width=0.95 * self.binwidth, color='k')

    def lineplot(self):
        plot(self.vals, self.histo)

def plot_circle(center,radius): # plot circles
```

```
    npoints = 100
    theta = arange(0,2*pi + 1e-7,2*pi/npoints)
    x = center[0] + radius*cos(theta)
    y = center[1] + radius*sin(theta)
    plot(x,y,'k',linewidth=2)

def draw_config(): # draw given configuration
    clf()
    for i in range(N):
        plot_circle(r[i, :], 0.5)
    axis('equal')
    gca().set_adjustable("box")
    view_scale = 4
    xlim(-view_scale, view_scale)
    ylim(-view_scale, view_scale)
    pause(0.01)

def init_config(): # initialize initial condition
    r = zeros((N, 2))
    n_side = int(sqrt(N) + 0.99)
    count = 0
    for row in range(n_side):
        for column in range(n_side):
            if count < N:
                r[count, :] = [row, column]
                count += 1
    return r

N = 7
delta_t = 0.01
total_time = 100
N_steps = int(total_time/delta_t)
T = 0.05
k_coll = 1 # collision rate

r = init_config()
v = zeros((N,2))
draw_config()

from numba import jit
@jit(nopython=True)
def compute_forces_and_potential(r): # compute energy and forces using␣
 ↪lj-potential
    forces = zeros((N,2))
    potential = 0
    for i in range(N):
        for j in range(i+1,N): # avoid self interaction
```

```
            dr = r[i,:] - r[j,:]
            dr2 = dr @ dr
            force_factor = 48 * ( dr2**(-7) - 0.5 * dr2**(-4) ) # force␣
 ↪magnitude (analytical derivative of lj potential)
            forces[i,:] += force_factor * dr # force on particle i
            forces[j,:] += force_factor * (-dr) # opposite force on particle j

            potential += 4 * ( dr2**(-6) - dr2**(-3) ) # lj potential

    return forces, potential

forces, potential_energy = compute_forces_and_potential(r)

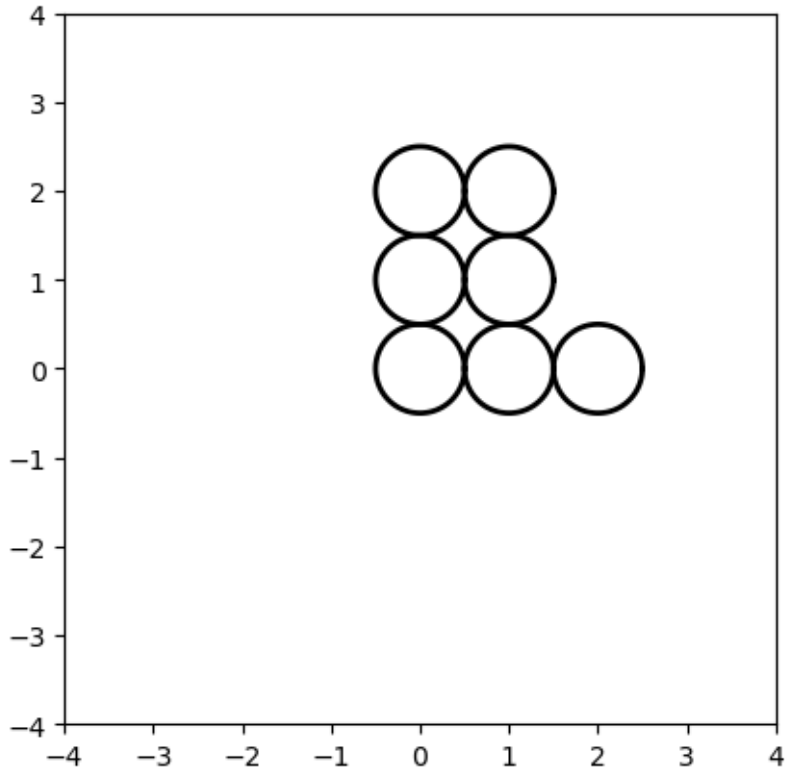
kinetic_traj = zeros(N_steps)
potential_traj = zeros(N_steps)
for step in range(N_steps): # simulation loop
    v = v + 0.5 * delta_t * forces # half velocity time step
    r = r + delta_t * v # full position time step
    forces, potential_energy = compute_forces_and_potential(r) # compute force␣
 ↪and potential
    v = v + 0.5 * delta_t * forces # other velocity half time step

    kinetic_energy = 0.5 * sum( v**2 )
    kinetic_traj[step] = kinetic_energy
    potential_traj[step] = potential_energy

    for i in range(N):
        if rand() < k_coll * delta_t: # metropolis MC condition, k_coll *␣
 ↪delta_t = probability of collision given time step
            speed = sqrt(-2 * T * log(rand()) ) # new speed drawn from␣
 ↪boltzmann dist
            angle = 2 * pi * rand() # new direction
            v[i,:] = speed * array([cos(angle), sin(angle)]) # assign new␣
 ↪random velocity

    if step % 1000 == 0:
        draw_config()

clf()
time_traj = arange(N_steps)*delta_t
plot(time_traj,kinetic_traj)
plot(time_traj,potential_traj)
plot(time_traj,kinetic_traj + potential_traj)
```


4
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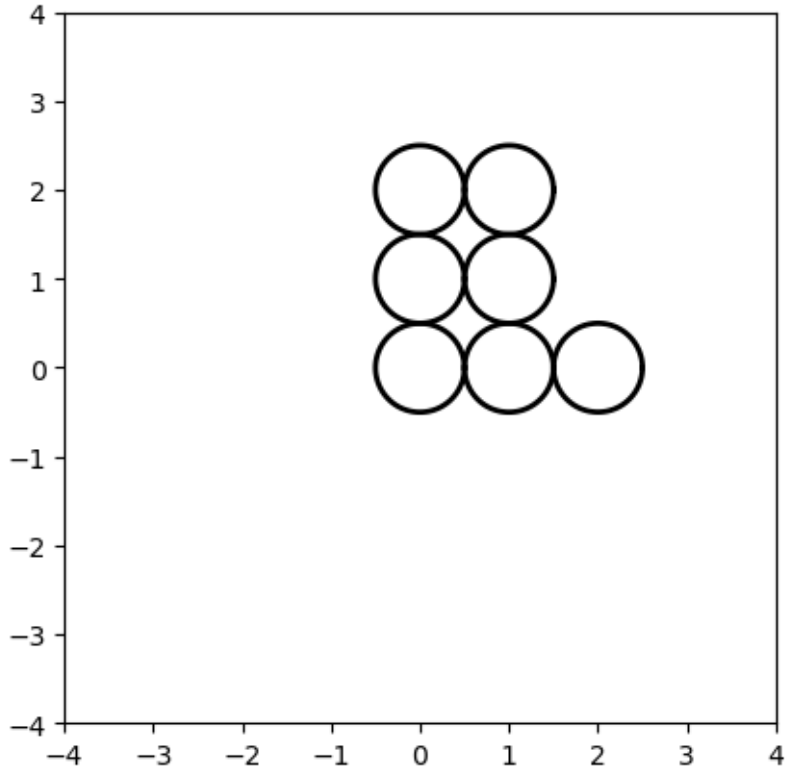
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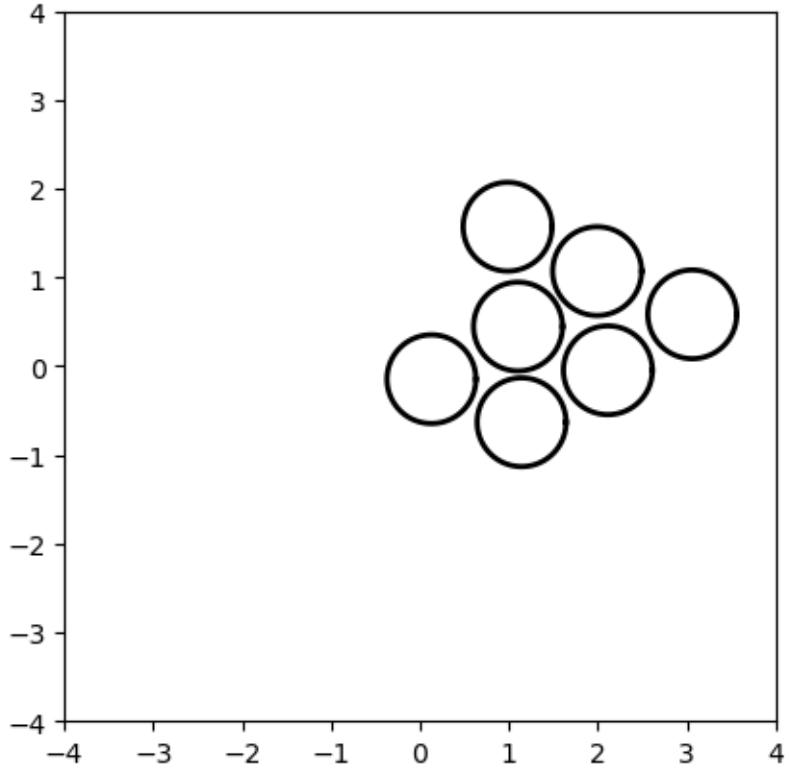
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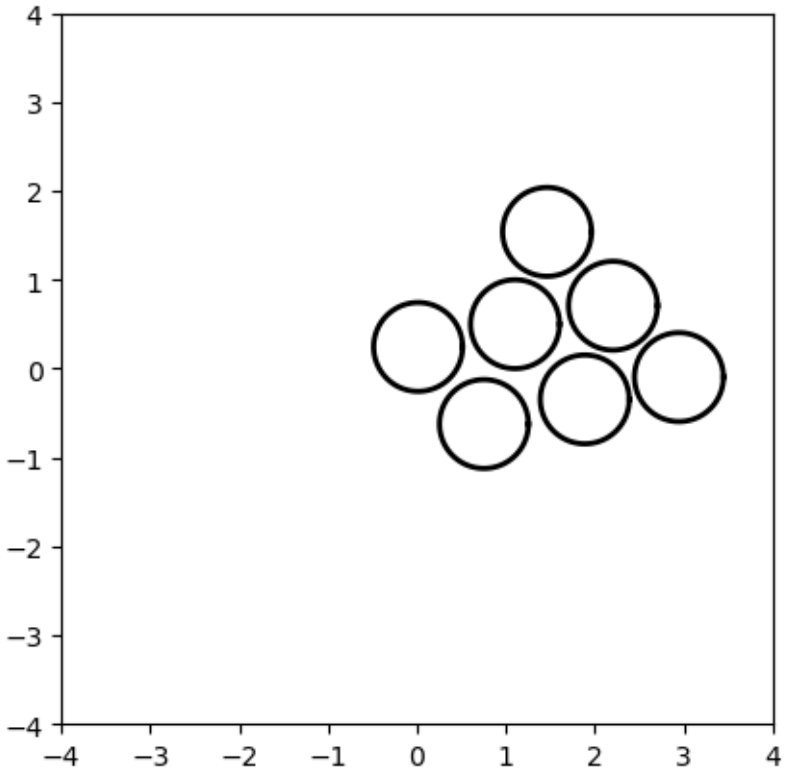
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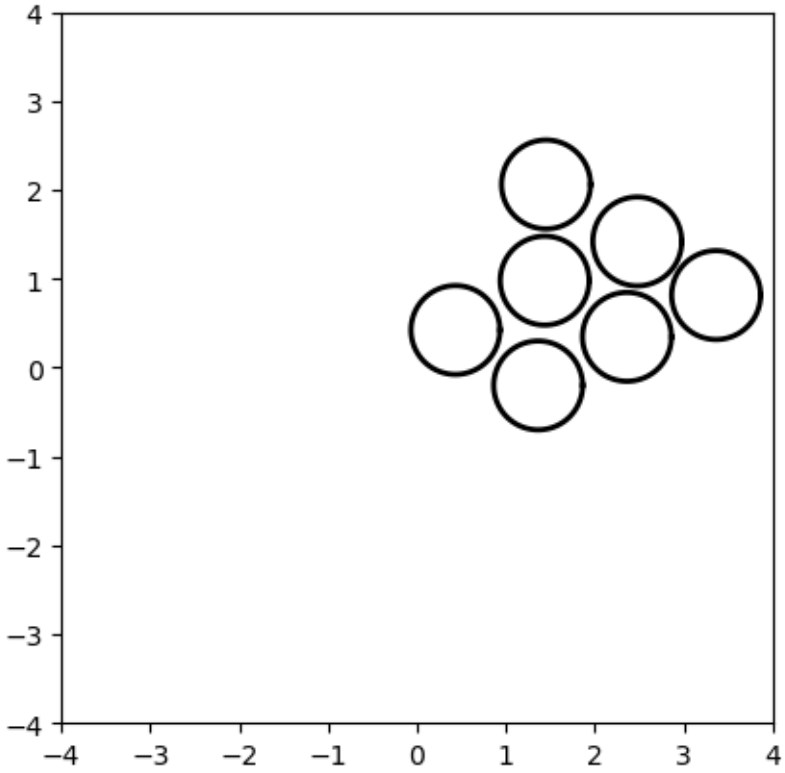
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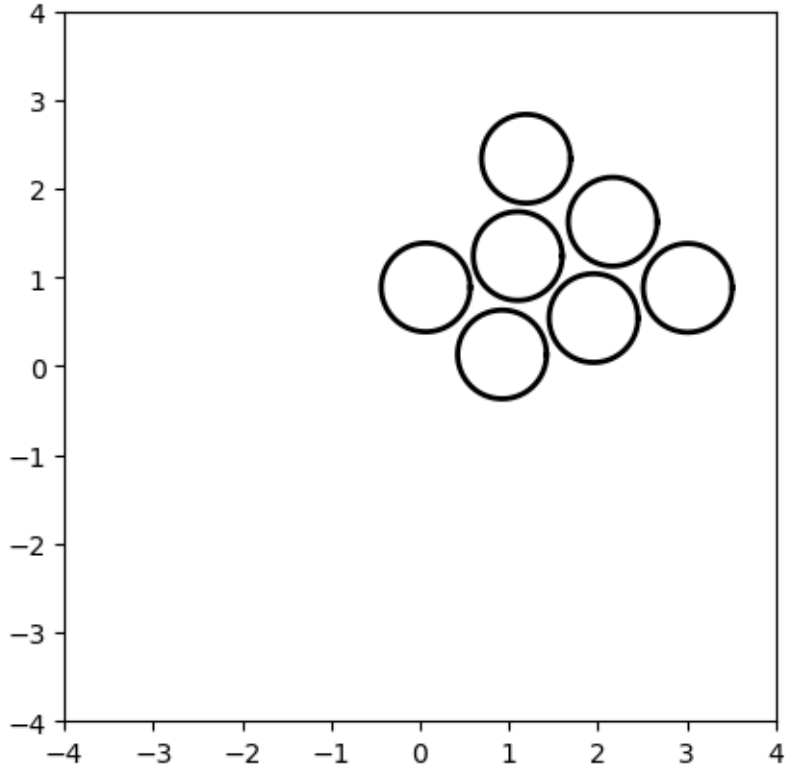
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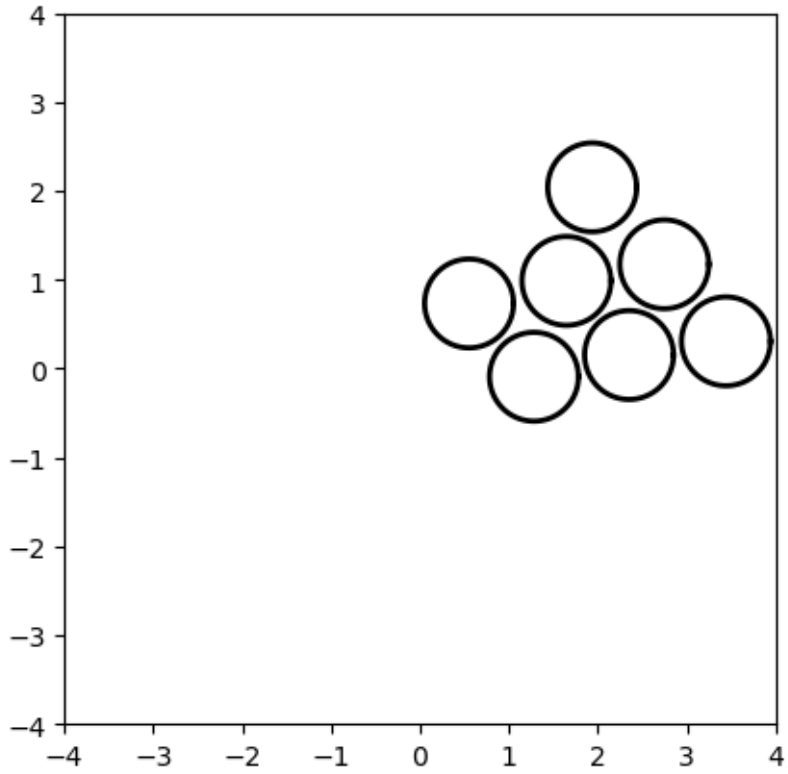
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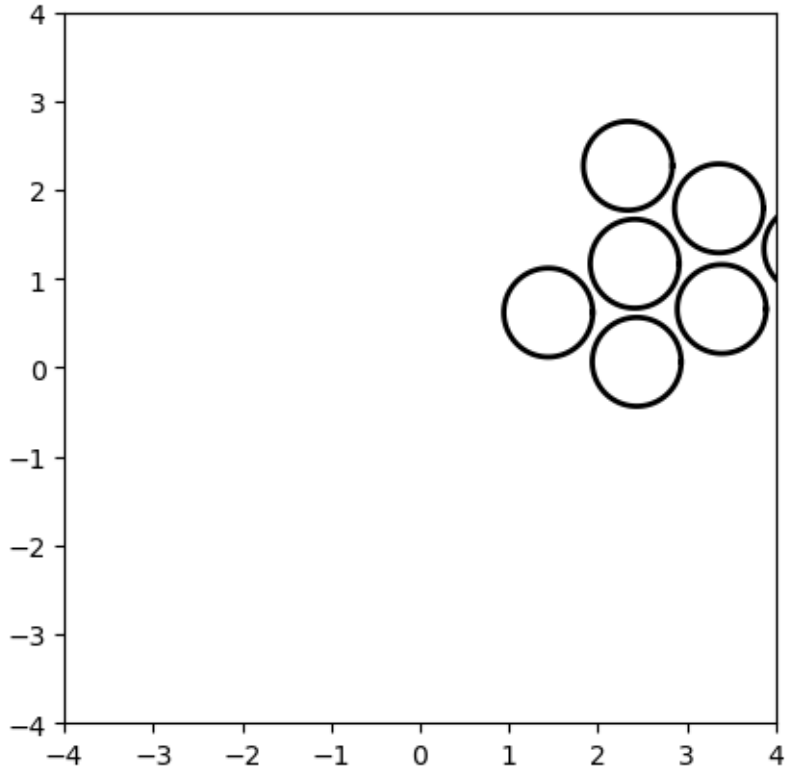
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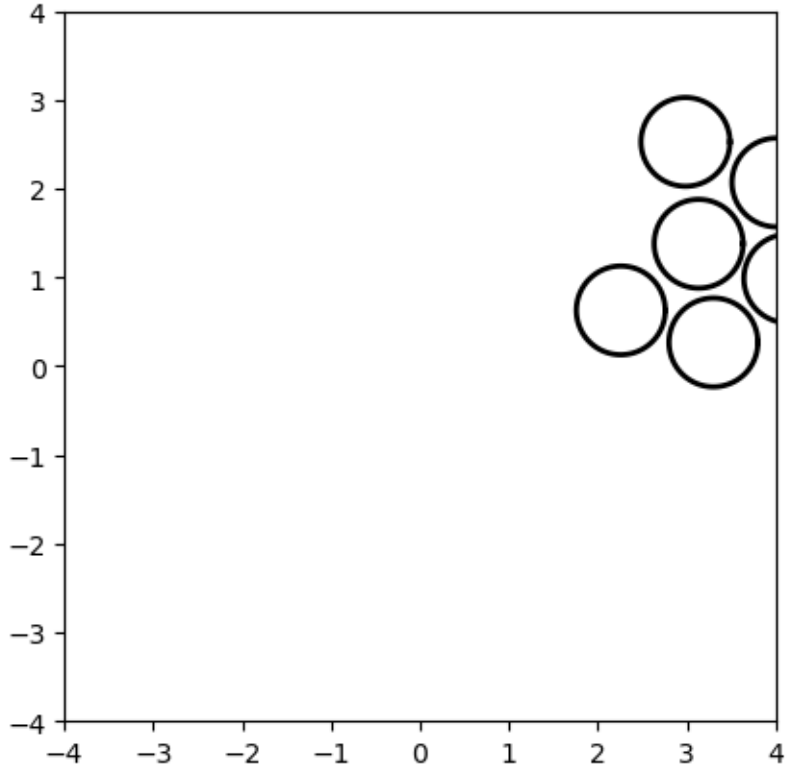
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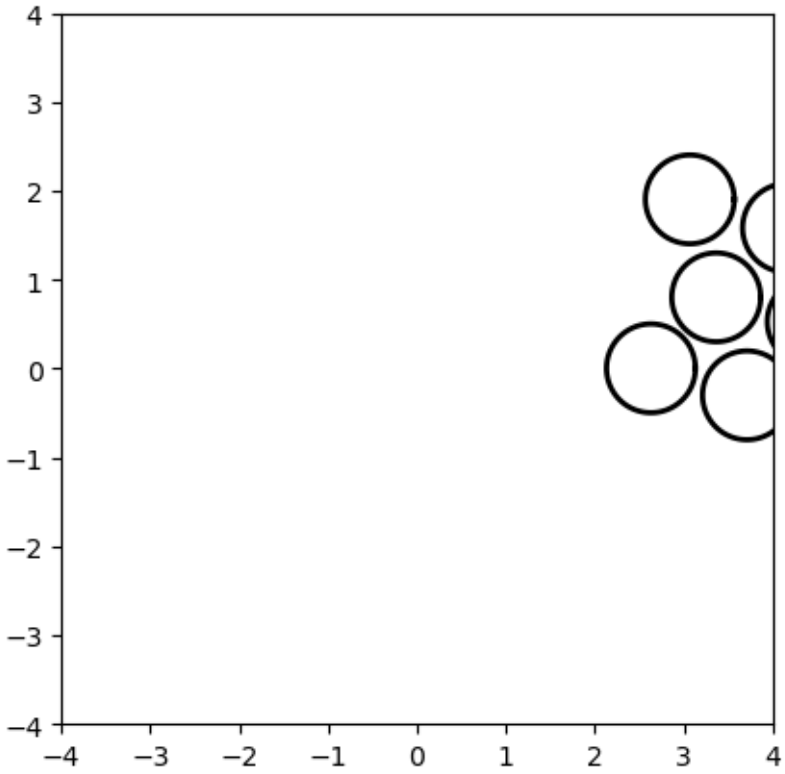
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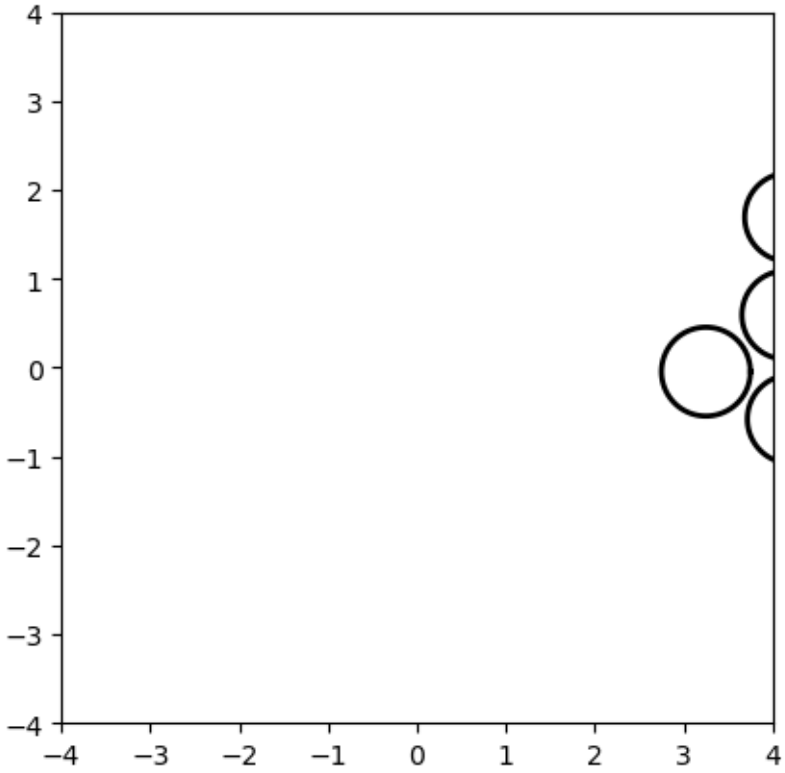
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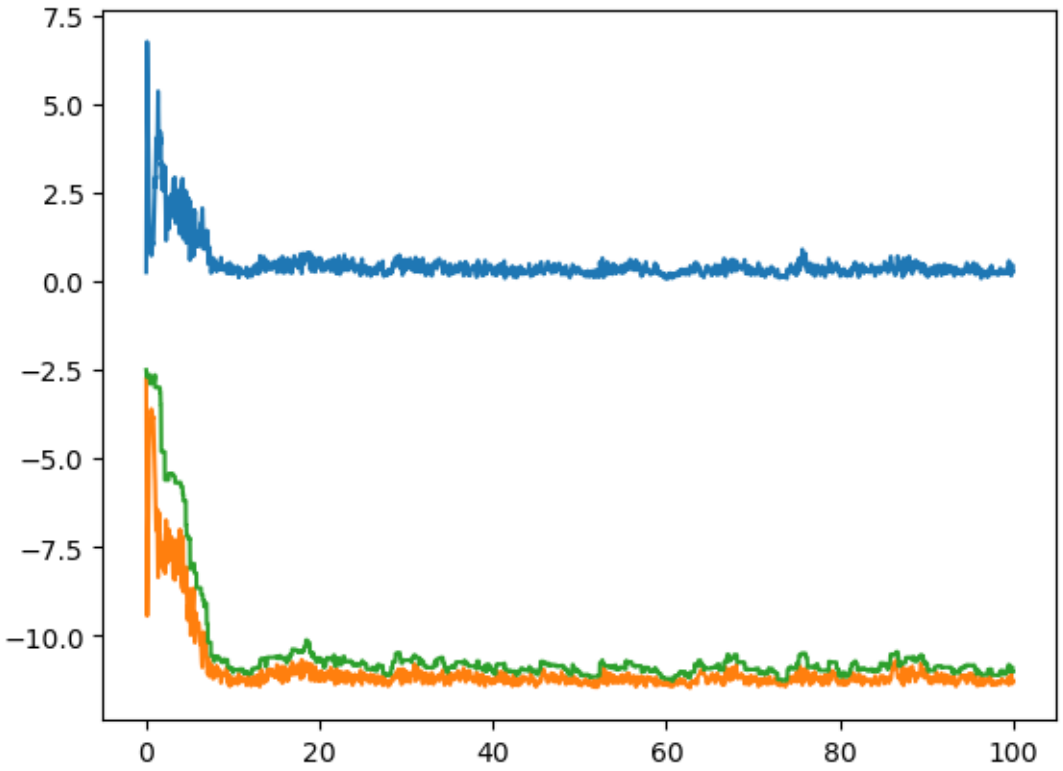
[2]: [<matplotlib.lines.Line2D at 0x30c98f550>]



1.2 (ii)

1.2.1 See Code

[41]:
```
N = 16
delta_t = 0.01
total_time = 100
N_steps = int(total_time/delta_t)
T = 0.05
k_coll = 1

density = 0.7
box_length = sqrt(N/density)
r_cut = box_length/2
r_cut_squared = r_cut**2

def init_config(N):
    r = zeros((N, 2))
```

```
    n_side = int(sqrt(N) + 0.99)
    count = 0
    for row in range(n_side):
        for column in range(n_side):
            if count < N:
                r[count, :] = [row, column]
                count += 1
    return r

def draw_config(N):
    clf()
    for i in range(N):
        plot_circle(r[i, :], 0.5)
    axis('equal')
    gca().set_adjustable("box")
    view_scale = 4
    xlim(-view_scale, view_scale)
    ylim(-view_scale, view_scale)
    pause(0.01)

r = init_config(N)
v = zeros((N,2))

@jit(nopython=True)
def compute_forces_and_potential(N, r, box_length):
    forces = np.zeros((N, 2))
    potential = 0.0
    for i in range(N):
        for j in range(i+1, N):
            dr = r[i,:] - r[j,:]
            dr -= box_length * np.floor(dr / box_length + 0.5)
            dr2 = dr @ dr

            if dr2 < r_cut_squared:
                # force_factor = 48 * (dr2**(-7) - 0.5 * dr2**(-4)) - 4 *␣
 ↪(r_cut_squared**(-7) - r_cut_squared**(-4))
                force_factor = 48 * (dr2**(-7) - 0.5 * dr2**(-4))

                forces[i,:] += force_factor * dr
                forces[j,:] -= force_factor * dr

                potential += 4 * (dr2**(-6) - dr2**(-3)) - 4 *␣
 ↪(r_cut_squared**(-6) - r_cut_squared**(-3))
    return forces, potential
```

```
forces, potential_energy = compute_forces_and_potential(N,r,box_length) # Force␣
 ↪and Potential Energy initialization

v = v + 0.5 * delta_t * forces # single time step update
r = r + delta_t * v
forces, potential_energy = compute_forces_and_potential(N,r,box_length)
v = v + 0.5 * delta_t * forces

for i in range(N):
    if rand() < k_coll * delta_t:
        speed = sqrt(-2 * T * log(rand()) )
        angle = 2 * pi * rand()
        v[i,:] = speed * array([cos(angle), sin(angle)])

print(f'U = {potential_energy}')
print(f'F_x = {forces[0]}')
```

```
U = -9.472133283012893
F_x = [-22.52238144 -22.52238144]
```

1.3 (iii)

1.3.1 See Code

[27]:
```
from tqdm import tqdm

N = 36
delta_t = 0.01
total_time = 1000
N_steps = int(total_time/delta_t)
T = 0.7
k_coll = 1

density = 0.7
box_length = sqrt(N/density)
r_cut = box_length/2
r_cut_squared = r_cut**2

r = init_config(N)
v = zeros((N,2))

binwidth = 0.05
g_r = histogram([0, 3.5], binwidth)
Mconf = 0

forces, potential_energy = compute_forces_and_potential(N,r,box_length)

kinetic_traj = zeros(N_steps)
```

```
potential_traj = zeros(N_steps)
for step in tqdm(range(N_steps)):
    v = v + 0.5 * delta_t * forces
    r = r + delta_t * v
    forces, potential_energy = compute_forces_and_potential(N,r,box_length)
    v = v + 0.5 * delta_t * forces

    kinetic_energy = 0.5 * sum( v**2 )
    kinetic_traj[step] = kinetic_energy
    potential_traj[step] = potential_energy

    for i in range(N):
        if rand() < k_coll * delta_t:
            speed = sqrt(-2 * T * log(rand()) )
            angle = 2 * pi * rand()
            v[i,:] = speed * array([cos(angle), sin(angle)])

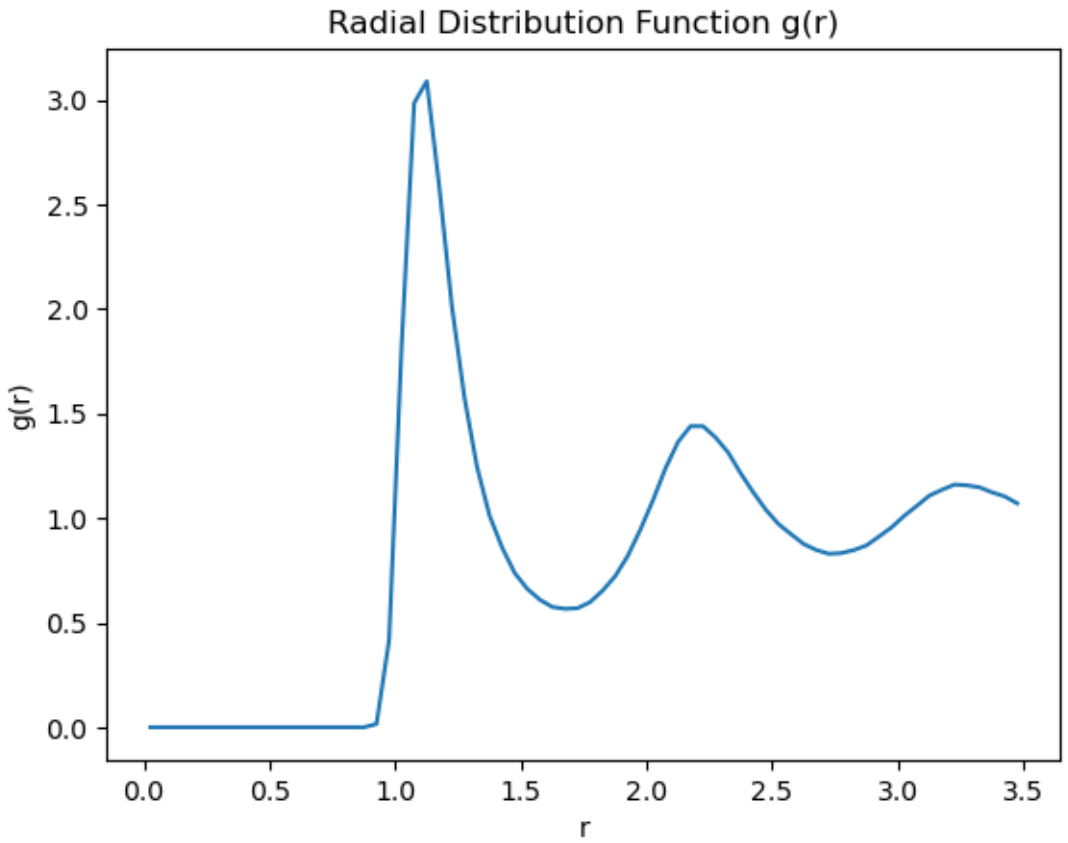
    # if step % 1000 == 0:
    #     draw_config()

    if step >= 10000 and step % 10 == 0: # 1000/0.01 = 100000 * 0.1 = 10000
        for i in range(N):
            for j in range(i + 1, N):
                dr_vec = r[i] - r[j]
                dr_vec -= box_length * floor(dr_vec / box_length + 0.5)
                distance = sqrt(dot(dr_vec, dr_vec))
                if distance < 3.5:
                    g_r.add_sample(distance)
        Mconf += 1


g_r.histo = g_r.histo / (Mconf * pi * g_r.vals * binwidth * (N - 1) * (N /␣
 ↪box_length**2))


g_r.lineplot()
xlabel('r')
ylabel('g(r)')
title('Radial Distribution Function g(r)')
show()
savefig('Visualizations/1_iii.png')
```

```
100%|
                    | 100000/100000 [00:35<00:00,
2830.49it/s]
```




```
<Figure size 640x480 with 0 Axes>
```

It aligns well with previous results. The characteristic oscillations in the particle density is visible.

2 Question 2

2.1 (i)

2.1.1 See Code

[42]:
```
def compute_virial_pressure(N, r, box_length, density):
    p_virial = density
    for i in range(N):
        for j in range(i + 1, N):
            dr = r[i,:] - r[j,:]
            dr -= box_length * floor(dr/box_length + 0.5)
            dr2 = dr @ dr
            if dr2 < r_cut_squared:
                p_virial += (24/box_length**2) * ( dr2**(-6) - 0.5 * dr2**(-3) )

    return p_virial
```

```
N = 36
delta_t = 0.01
total_time = 1000
N_steps = int(total_time/delta_t)
T = 0.7
k_coll = 1

density = 0.7
box_length = sqrt(N/density)
r_cut = box_length/2
r_cut_squared = r_cut**2

r = init_config(N)

compute_virial_pressure(N, r, box_length, density)
```

[42]: np.float64(13.180280002043103)

2.2 (ii)

2.2.1 See Code

[29]:
```
from tqdm import tqdm

N = 36
delta_t = 0.01
total_time = 100
N_steps = int(total_time/delta_t)
T = 0.7
k_coll = 1

density = 0.7
box_length = sqrt(N/density)
r_cut = box_length/2
r_cut_squared = r_cut**2

r = init_config(N)
v = zeros((N,2))

forces, potential_energy = compute_forces_and_potential(N,r,box_length)

kinetic_traj = zeros(N_steps)
potential_traj = zeros(N_steps)
p_virials = []

for step in tqdm(range(N_steps)):
    v = v + 0.5 * delta_t * forces
```

```
    r = r + delta_t * v
    forces, potential_energy = compute_forces_and_potential(N,r,box_length)
    v = v + 0.5 * delta_t * forces

    kinetic_energy = 0.5 * sum( v**2 )
    kinetic_traj[step] = kinetic_energy
    potential_traj[step] = potential_energy

    for i in range(N):
        if rand() < k_coll * delta_t:
            speed = sqrt(-2 * T * log(rand()) )
            angle = 2 * pi * rand()
            v[i,:] = speed * array([cos(angle), sin(angle)])

    # if step % 1000 == 0:
    #     draw_config()

    if step >= 1000 and step % 10 == 0:
        p_virials.append(compute_virial_pressure(N, r, box_length, density))

print(f'average virial pressure: {np.mean(p_virials)}')
```

```
100%|
                          | 10000/10000 [00:03<00:00,
3072.18it/s]
average virial pressure: 1.0701850144737148
```

2.3 (iii)

[35]:
```
from tqdm import tqdm

N = 36
delta_t = 0.01
total_time = 100
N_steps = int(total_time/delta_t)
T = 0.7
k_coll = 1

densitys = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8]
p_virialss = []

for density in densitys:
    box_length = sqrt(N/density)
    r_cut = box_length/2
```

```
    r_cut_squared = r_cut**2

    r = init_config(N)
    v = zeros((N,2))
    forces, potential_energy = compute_forces_and_potential(N,r,box_length)

    kinetic_traj = zeros(N_steps)
    potential_traj = zeros(N_steps)

    p_virials = []
    for step in tqdm(range(N_steps)):
        v = v + 0.5 * delta_t * forces
        r = r + delta_t * v
        forces, potential_energy = compute_forces_and_potential(N,r,box_length)
        v = v + 0.5 * delta_t * forces

        kinetic_energy = 0.5 * sum( v**2 )
        kinetic_traj[step] = kinetic_energy
        potential_traj[step] = potential_energy

        for i in range(N):
            if rand() < k_coll * delta_t:
                speed = sqrt(-2 * T * log(rand()) )
                angle = 2 * pi * rand()
                v[i,:] = speed * array([cos(angle), sin(angle)])

        # if step % 1000 == 0:
        #     draw_config()

        if step >= 1000 and step % 10 == 0:
            p_virials.append(compute_virial_pressure(N, r, box_length, density))

    p_virialss.append(np.mean(p_virials))
```

```
100%|

                      | 10000/10000 [00:02<00:00,
3377.32it/s]
100%|

                      | 10000/10000 [00:02<00:00,
3373.49it/s]
100%|

                      | 10000/10000 [00:03<00:00,
3285.12it/s]
100%|
```

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                        | 10000/10000 [00:03<00:00,
3307.53it/s]
100%|

                        | 10000/10000 [00:03<00:00,
3250.61it/s]
100%|

                        | 10000/10000 [00:03<00:00,
3178.48it/s]
100%|

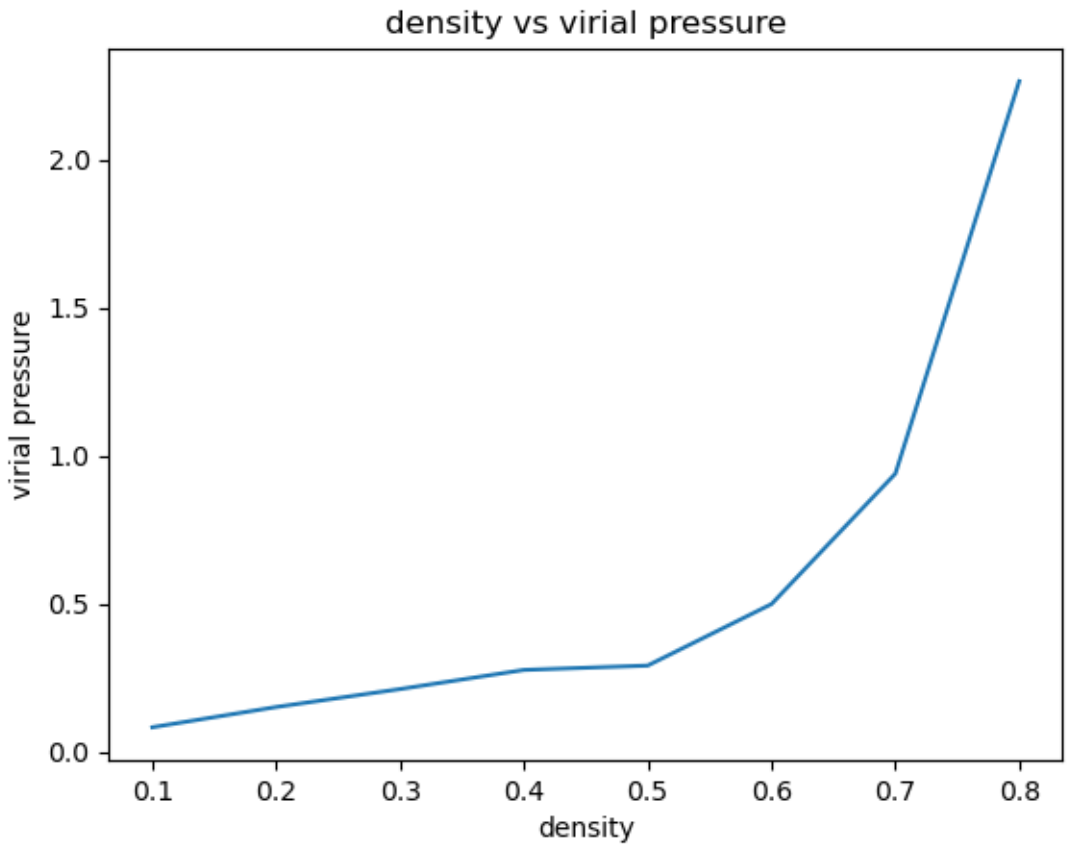
                        | 10000/10000 [00:03<00:00,
3105.47it/s]
100%|

                        | 10000/10000 [00:03<00:00,
3072.58it/s]
```

[36]:
```
p_virialss
```

[36]:
```
[np.float64(0.08285965268579802),
 np.float64(0.15121404252867898),
 np.float64(0.21181263385466562),
 np.float64(0.27644514312078444),
 np.float64(0.29121007309994695),
 np.float64(0.4990417389889261),
 np.float64(0.9394817902478239),
 np.float64(2.264946207039888)]
```

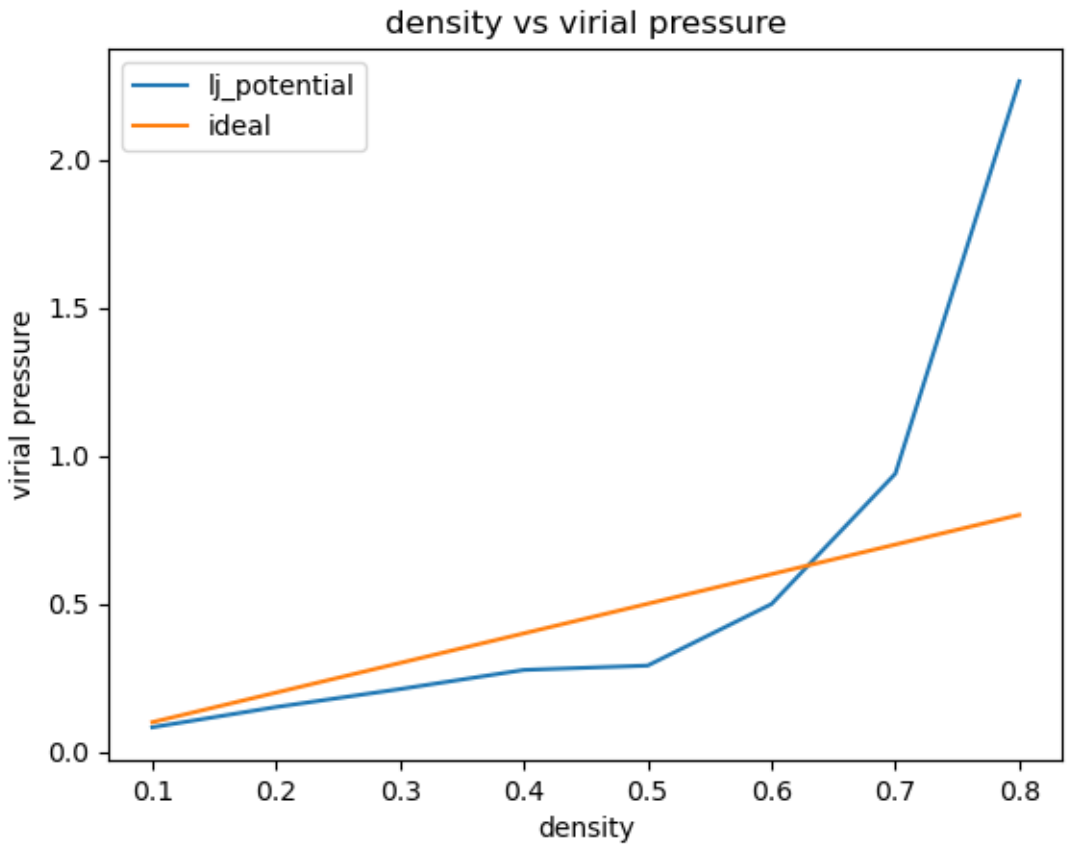
[37]:
```
clf()
plot(densitys,p_virialss)
xlabel('density')
ylabel('virial pressure')
title('density vs virial pressure')
show()
savefig('Visualizations/2_iii.png')
```




```
<Figure size 640x480 with 0 Axes>
```

2.4 (iv)

[38]:
```
clf()
time_traj = arange(N_steps - 1000)*delta_t
plot(densitys,p_virialss, label='lj_potential')
plot(densitys, densitys, label='ideal')
xlabel('density')
ylabel('virial pressure')
title('density vs virial pressure')
legend()
show()
savefig('Visualizations/2_iv.png')
```




```
<Figure size 640x480 with 0 Axes>
```

The LJ potential is stabilizing by a r^{-6} scale, causing a more attractive force and therefore decreasing the virial pressure. This is stabilization increases as more particles are present. However, after a certain interparticle distance or particle density, the LJ potential becomes destabilizing by a r^{-12} scale, causing an additional repulsive force, increasing the virial pressure. The plot above shows this trend, where lower densities correspond to lower than idea virial pressures while very high densities correspond diverging virial pressure.

2.5 (v)

2.5.1 See Code

[43]:
```
from tqdm import tqdm

N = 36
delta_t = 0.01
total_time = 100
N_steps = int(total_time/delta_t)
T = 0.7
k_coll = 1
```

```
densitys = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8]
p_virialss = []

for density in densitys:
    box_length = sqrt(N/density)
    r_cut = 2**(1/6)
    r_cut_squared = r_cut**2

    r = init_config(N)
    v = zeros((N,2))
    forces, potential_energy = compute_forces_and_potential(N,r,box_length)

    kinetic_traj = zeros(N_steps)
    potential_traj = zeros(N_steps)

    p_virials = []
    for step in tqdm(range(N_steps)):
        v = v + 0.5 * delta_t * forces
        r = r + delta_t * v
        forces, potential_energy = compute_forces_and_potential(N,r,box_length)
        v = v + 0.5 * delta_t * forces

        kinetic_energy = 0.5 * sum( v**2 )
        kinetic_traj[step] = kinetic_energy
        potential_traj[step] = potential_energy

        for i in range(N):
            if rand() < k_coll * delta_t:
                speed = sqrt(-2 * T * log(rand()) )
                angle = 2 * pi * rand()
                v[i,:] = speed * array([cos(angle), sin(angle)])

        # if step % 1000 == 0:
        #     draw_config()

        if step >= 1000 and step % 10 == 0:
            p_virials.append(compute_virial_pressure(N, r, box_length, density))

    p_virialss.append(np.mean(p_virials))
```

```
100%|
                        | 10000/10000 [00:02<00:00,
3594.50it/s]
100%|
                        | 10000/10000 [00:02<00:00,
```

```
3529.91it/s]
100%|

                          | 10000/10000 [00:02<00:00,
3515.88it/s]
100%|

                          | 10000/10000 [00:02<00:00,
3405.04it/s]
100%|

                          | 10000/10000 [00:02<00:00,
3387.56it/s]
100%|

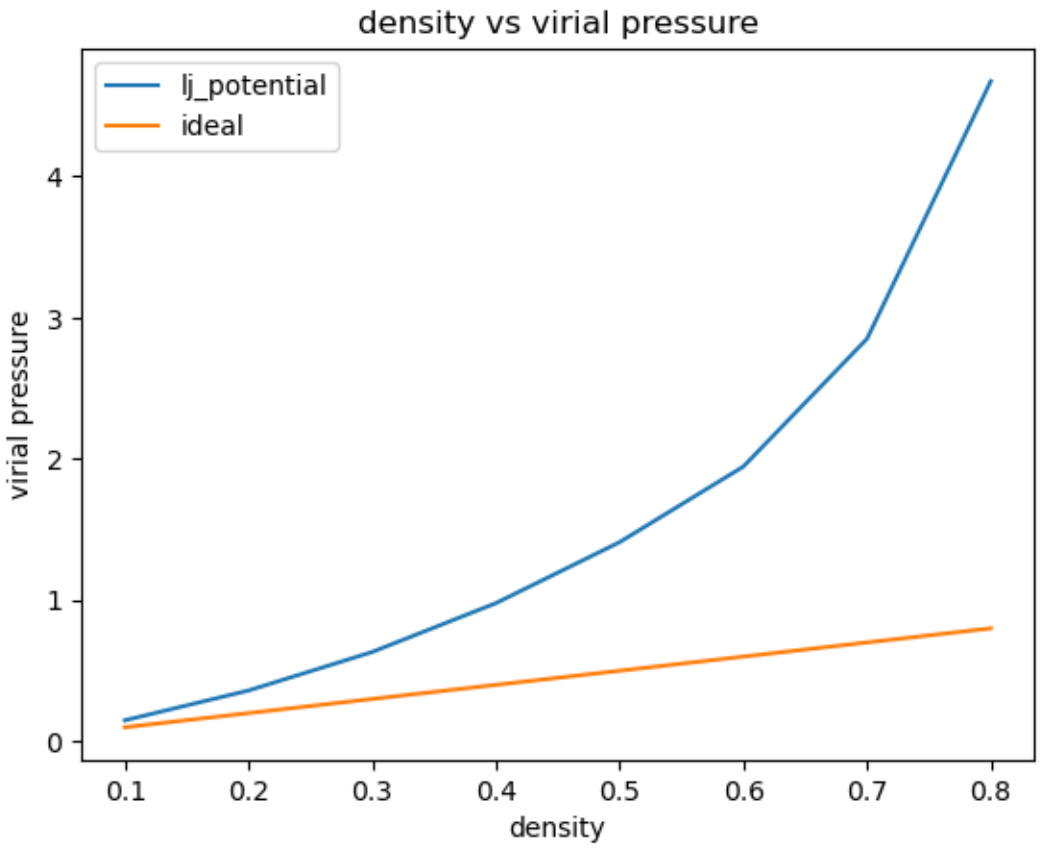
                          | 10000/10000 [00:02<00:00,
3365.12it/s]
100%|

                          | 10000/10000 [00:03<00:00,
3232.25it/s]
100%|

                          | 10000/10000 [00:03<00:00,
3214.09it/s]
```

2.6 (vi)

[44]:
```
clf()
time_traj = arange(N_steps - 1000)*delta_t
plot(densitys,p_virialss, label='lj_potential')
plot(densitys, densitys, label='ideal')
xlabel('density')
ylabel('virial pressure')
title('density vs virial pressure')
legend()
show()
savefig('Visualizations/2_v.png')
```




```
<Figure size 640x480 with 0 Axes>
```

With a smaller cutoff radius, the stabalizing energy is removed and only the destabilizing portion remains. Without the stabalizing interaction energy, the new virial pressure resembles the ideal gas at smaller densities, but should diverge more significantly at higher densities.