ex01

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Numerical Methods in Plasma Astrophysics

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Exercise 1: N-Body Rubber Ducks

[121]:
```
import time
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.animation import FuncAnimation
%matplotlib inline

np.random.seed(0)

def Calculate_Temperature(vel,N):
    real_vel = vel.copy()
    v_squared = np.sum(real_vel*real_vel, axis=1)
    v_mean = np.mean(v_squared)
    ene_kin_aver = 0.5*v_mean
    temperature = ene_kin_aver/3
    return ene_kin_aver,temperature


def compute_force(x):
    rm = 2
    n = x.shape[0]
    a = np.zeros(x.shape)
    energy_pot = np.zeros(x.shape)
    for i in range(n):
        for j in range(n):
            if i==j:
                continue
            r_vec = x[i] - x[j]
            for l in range(2): # Periodic interactions
                if (np.abs(r_vec[l])>10):
                    r_vec[l] = r_vec[l] - np.copysign(20.0,r_vec[l])
            r = np.sqrt(r_vec@r_vec)
            if (r<10):
```

```
                phi = (rm/r)**12 - 2*(rm/r)**6
                dphi = 12*rm**12/r**14 - 12*rm**6/r**8
                a[i] += dphi*r_vec
                a[j] -= dphi*r_vec
                energy_pot[i] += 0.5*phi
                energy_pot[j] += 0.5*phi
    return a, np.mean(energy_pot)


def solve_nbody(x, v, mu, dt, steps, method):
    n = x.shape[0]
    traj = np.zeros((steps, n, 2))
    temps = np.zeros(steps)
    energy_kin = np.zeros(steps)
    energy_pot = np.zeros(steps)

    for s in range(steps):
        for i in range(2):
            period = np.where(x[:,i] > 10)
            x[period,i]=x[period,i]-20
            period = np.where(x[:,i] < -10)
            x[period,i]=x[period,i]+20
        if method=="Leapfrog":
            x_half = x + v*dt/2
            a, energy_pot[s] = compute_force(x_half)
            energy_kin[s],temps[s] = Calculate_Temperature(v, n)
            v = v + (a - mu*v)*dt
            x = x_half + dt/2*v
        if method=="Euler":
            x = x + v*dt
            a, energy_pot[s] = compute_force(x)
            energy_kin[s],temps[s] = Calculate_Temperature(v, n)
            v = v + a*dt
        traj[s] = x
    return traj, energy_kin, energy_pot, temps
```

a) Development of rubber duck population

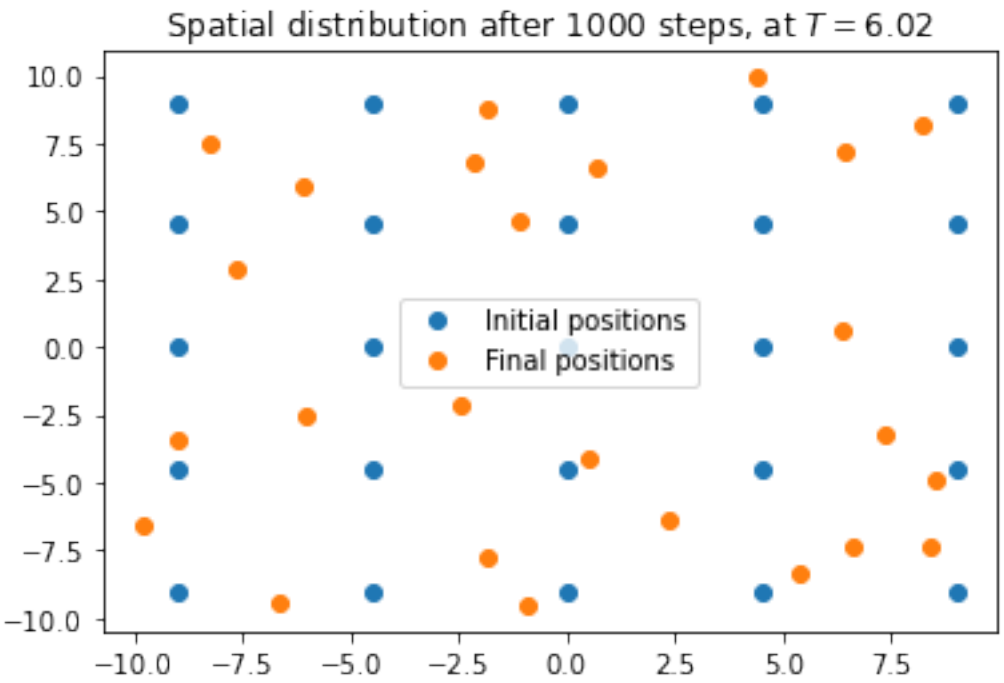
The temperature is dependend on the standard deviation of the velocity distribution, so starting with different standard deviation is equivalent to starting with different temperatures

[91]:
```
n = 5**2
mu = 0.0
dt = 0.01
steps = 1000
boxsize = 10
```

```
lin = np.linspace(-9,9,int(np.sqrt(n)))
X,Y = np.meshgrid(lin,lin)

x = np.vstack([X.ravel(), Y.ravel()]).T
```

[93]:
```
v = np.random.normal(0,5.0,(n,2))
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
 ↪"Leapfrog")
plt.plot(x[:,0], x[:,1], "o", label="Initial positions")
plt.plot(traj[-1,:,0], traj[-1,:,1],"o", label="Final positions")
plt.title("Spatial distribution after {} steps, at $T=${:.2f}".format(steps,␣
 ↪temps[-1]))
plt.legend()
```

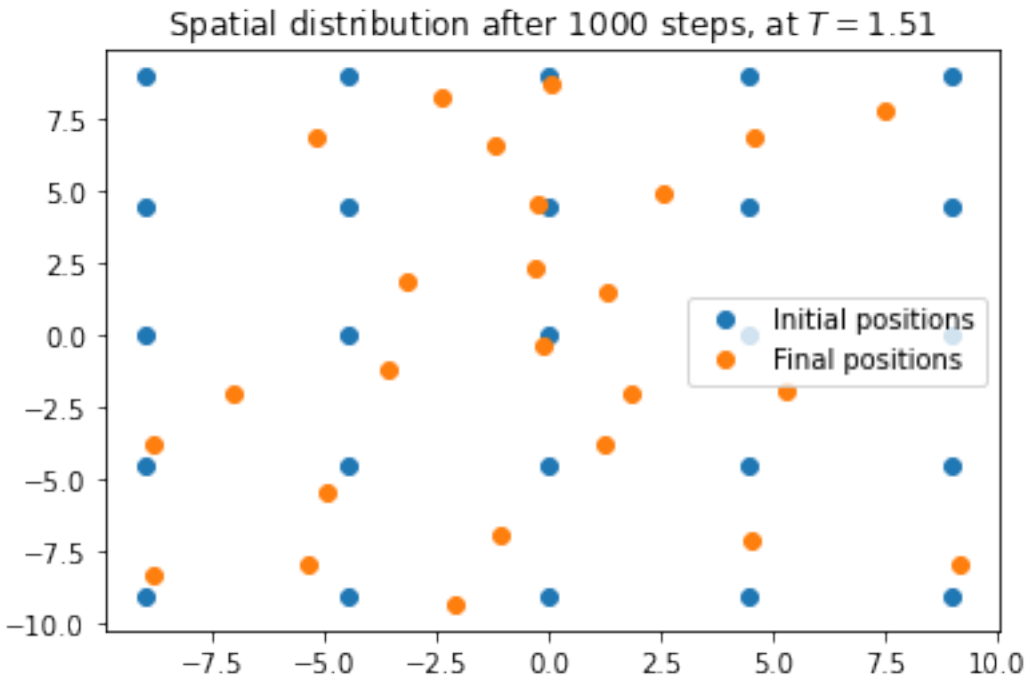
[93]: <matplotlib.legend.Legend at 0x7fc4a6798190>



[94]:
```
v = np.random.normal(0,2.0,(n,2))
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
 ↪"Leapfrog")
plt.plot(x[:,0], x[:,1], "o", label="Initial positions")
plt.plot(traj[-1,:,0], traj[-1,:,1],"o", label="Final positions")
plt.title("Spatial distribution after {} steps, at $T=${:.2f}".format(steps,␣
 ↪temps[-1]))
```

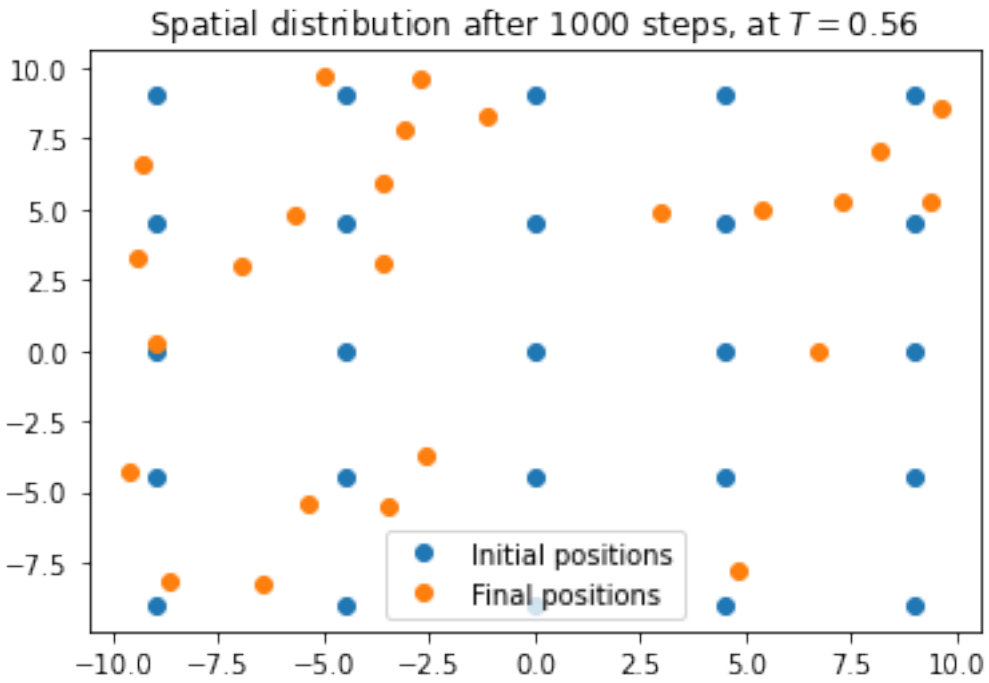
```
plt.legend()
```

[94]: <matplotlib.legend.Legend at 0x7fc4a6af5160>



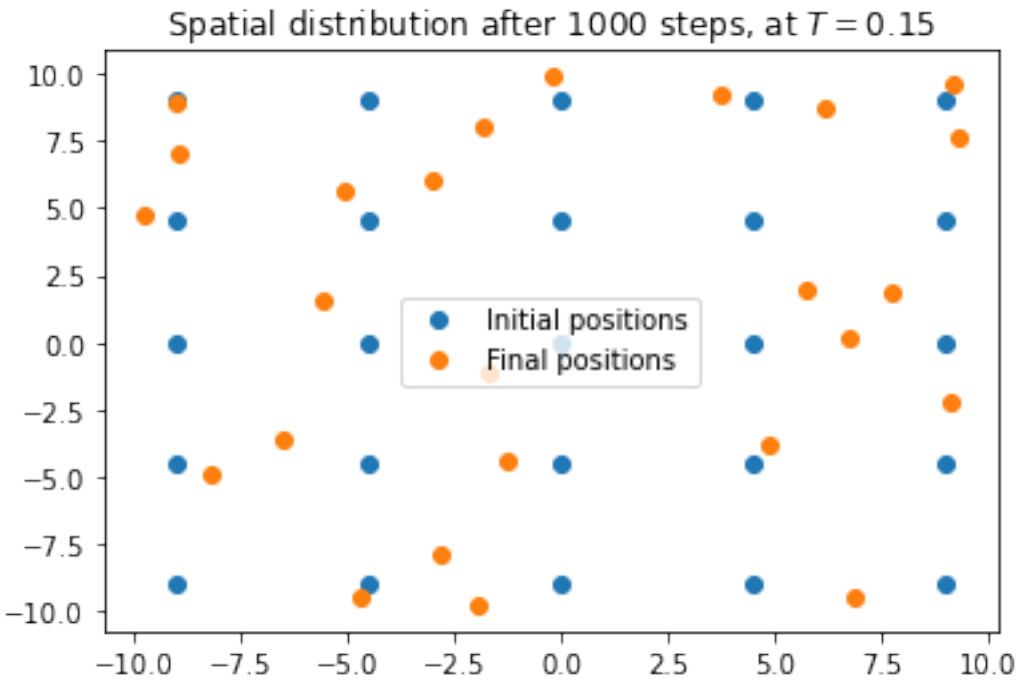
[95]:
```
v = np.random.normal(0,1.0,(n,2))
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
↪"Leapfrog")
plt.plot(x[:,0], x[:,1], "o", label="Initial positions")
plt.plot(traj[-1,:,0], traj[-1,:,1],"o", label="Final positions")
plt.title("Spatial distribution after {} steps, at $T=${:.2f}".format(steps,␣
↪temps[-1]))
plt.legend()
```

[95]: <matplotlib.legend.Legend at 0x7fc4a6c28670>



[96]:
```
v = np.random.normal(0,0.1,(n,2))
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
 ↪"Leapfrog")
plt.plot(x[:,0], x[:,1], "o", label="Initial positions")
plt.plot(traj[-1,:,0], traj[-1,:,1],"o", label="Final positions")
plt.title("Spatial distribution after {} steps, at $T=${:.2f}".format(steps,␣
 ↪temps[-1]))
plt.legend()
```

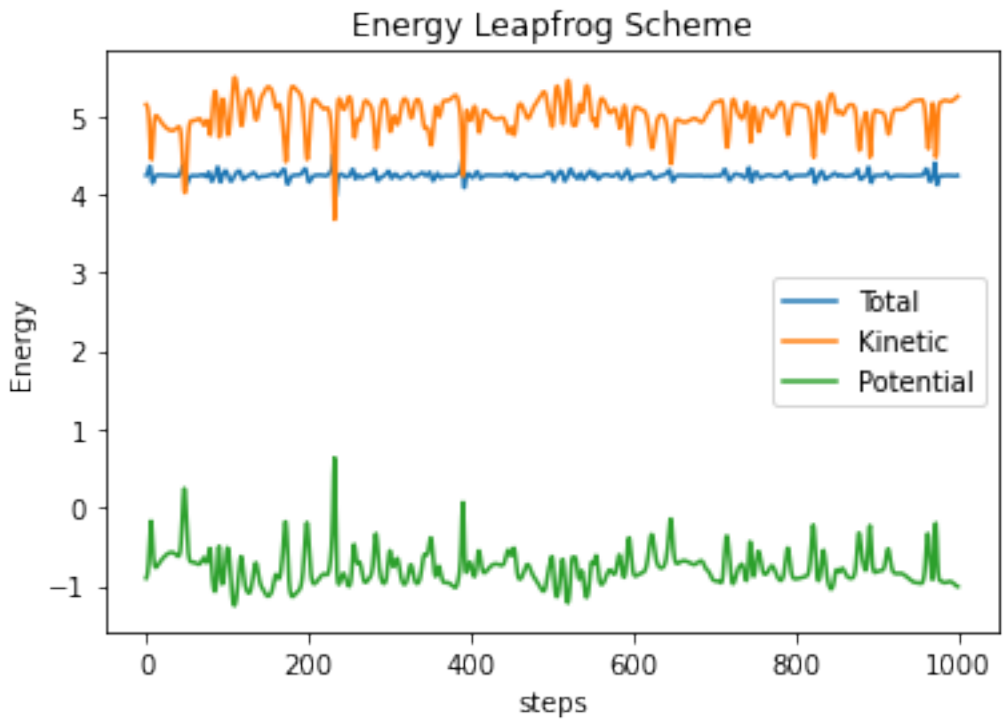
[96]:
```
<matplotlib.legend.Legend at 0x7fc4a6856df0>
```



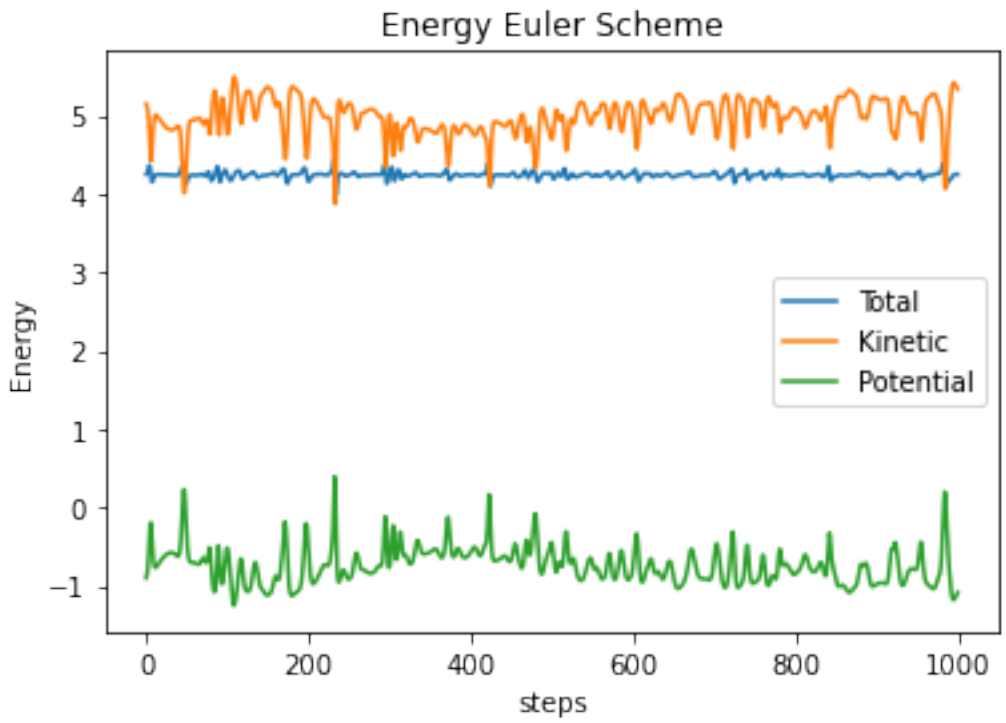
For high temperatures, no pattern in the arrangement of the particles can be observed. However, with decreasing temperature we can see a progressive formation of clusters of particles which "stick" together. At lowest temperature the particles are making chains and crystal-like structures.

b) Total energy developement

[86]:
```
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
↪"Leapfrog")
plt.plot((energy_kin+energy_pot), label="Total")
plt.plot(energy_kin, label="Kinetic")
plt.plot(energy_pot, label="Potential")
plt.title("Energy Leapfrog Scheme")
plt.xlabel("steps")
plt.ylabel("Energy")
plt.legend()
plt.show()
```



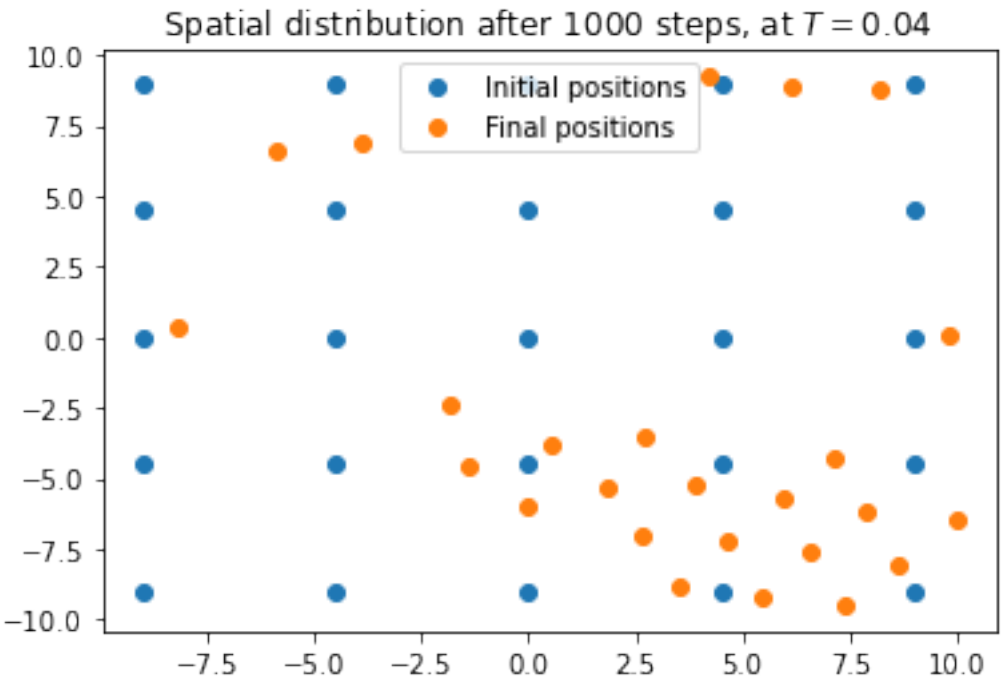
[87]:
```
traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps, "Euler")
plt.plot((energy_kin+energy_pot), label="Total")
plt.plot(energy_kin, label="Kinetic")
plt.plot(energy_pot, label="Potential")
plt.title("Energy Euler Scheme")
plt.xlabel("steps")
plt.ylabel("Energy")
plt.legend()
plt.show()
```



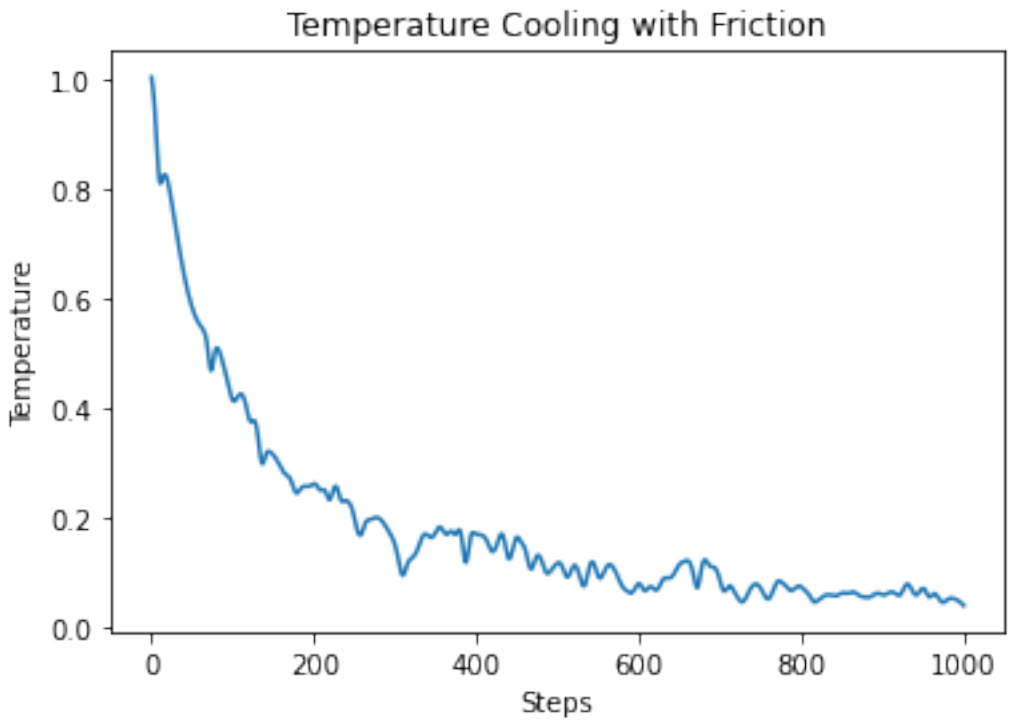
The total energy, the sum of kinetic and potential energy, stays more or less constant over time as expected for a energy conserving system. The Leapfrog scheme seems to perform slightly better than the Euler schmeme, which tends to have bigger oscilattions in the energies.

c) Cooling

[100]:
```
mu = 0.5
v = np.random.normal(0,2.0,(n,2))

traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
↪"Leapfrog")

plt.plot(x[:,0], x[:,1], "o", label="Initial positions")
plt.plot(traj[-1,:,0], traj[-1,:,1],"o", label="Final positions")
plt.title("Spatial distribution after {} steps, at $T=${:.2f}".format(steps,␣
↪temps[-1]))
plt.legend()
plt.show()
```



[101]:
```
plt.title("Temperature Cooling with Friction")
plt.plot(temps)
plt.xlabel("Steps")
plt.ylabel("Temperature")
plt.show()
```



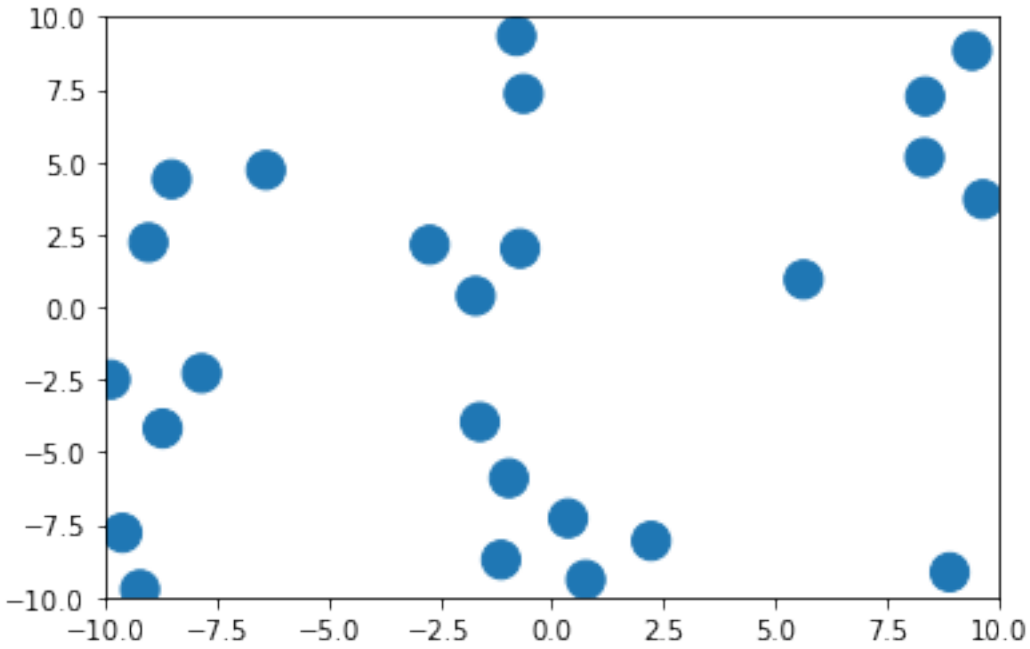
As the temperature falls, the ducks start to make crystal like patters (hexagonal in our case, because of optimal distribution in a plane). This is because the lennard-jones potential has a minimum, the preferred distance r_m.

Additional: Animation of the crystal formation when cooling down the system

[17]:
```
fig = plt.figure()
ax = plt.axes(xlim=(-10, 10), ylim=(-10, 10))

n = 10
v = np.random.normal(0,1,(n,2))
x = np.random.uniform(0,10,(n,2))

line = ax.scatter(traj[0,:,0], traj[0,:,1], s=np.ones(traj[0,:,0].shape)*200)

dt = 0.01
def init():
    line.set_offsets(np.c_[x[:,0], x[:,1]])
    return line,
def animate(i):
    x = traj[i]
    line.set_offsets(np.c_[x[:,0], x[:,1]])
```

```
    return line,

anim = FuncAnimation(fig, animate, frames=1000, interval=20)
anim.save('lennard_jones_cooling.gif',writer='imagemagick')
```

```
MovieWriter imagemagick unavailable; using Pillow instead.
```



1 d) Plot of Runtime for Euler and Leapfrog

[109]:
```
def eval_time(n):
    #n = 5**2
    mu = 0.0
    dt = 0.01
    steps = 10
    boxsize = 10

    lin = np.linspace(-9,9,int(np.sqrt(n)))
    X,Y = np.meshgrid(lin,lin)

    x = np.vstack([X.ravel(), Y.ravel()]).T
    v = np.random.normal(0,0.1,(n,2))

    start_time = time.time()
```

```
    traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
↪"Leapfrog")
    end_time = time.time()
    time_lf = end_time - start_time

    start_time = time.time()
    traj, energy_kin, energy_pot, temps = solve_nbody(x, v, mu, dt, steps,␣
↪"Euler")
    end_time = time.time()
    time_euler = end_time - start_time

    return np.array([time_lf, time_euler])
```

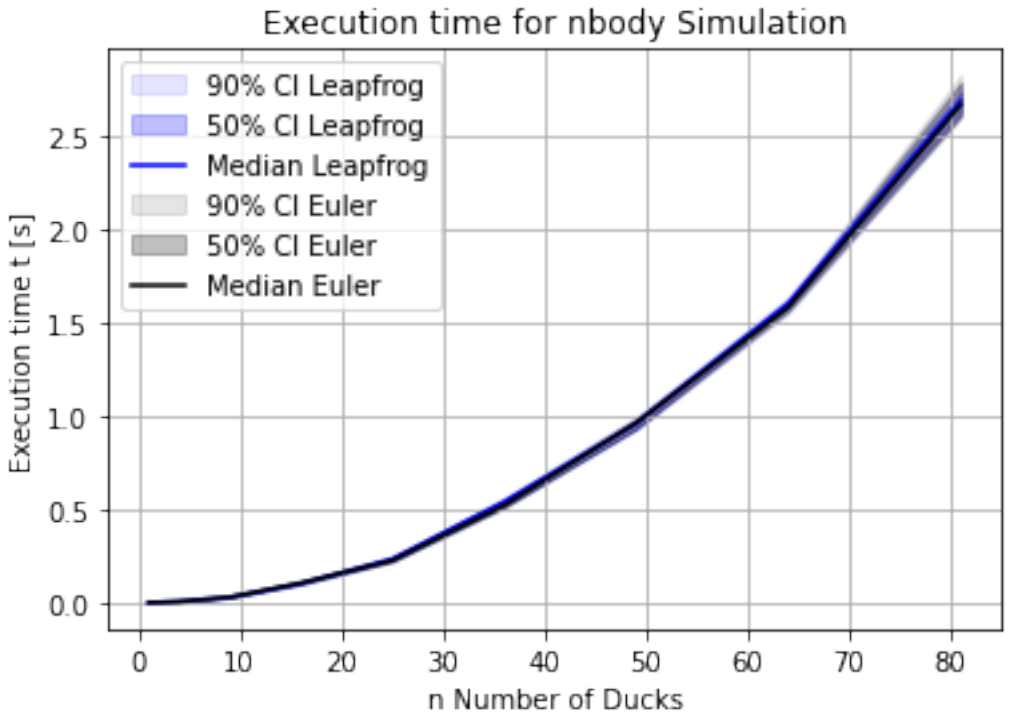
[113]:
```
ns = [i**2 for i in range(1,10)]
times = []
repeat = 10
print(repeat)
for i in range(repeat):
    print("Current round:", i)
    times.append(np.array([eval_time(n) for n in ns]))

times = np.array(times)
times_lf = times[:,:,0]
times_euler = times[:,:,1]
```

```
10
Current round: 0
Current round: 1
Current round: 2
Current round: 3
Current round: 4
Current round: 5
Current round: 6
Current round: 7
Current round: 8
Current round: 9
```

[122]:
```
plt.fill_between(ns, np.percentile(times_lf, axis=0, q=[10]).ravel()[:],
                     np.percentile(times_lf, axis=0, q=[90]).ravel()[:],
                     alpha = 0.1, color='b', label='90% CI Leapfrog');

plt.fill_between(ns, np.percentile(times_lf, axis=0, q=[25]).ravel()[:],
                     np.percentile(times_lf, axis=0, q=[75]).ravel()[:],
                     alpha = 0.25, color='b', label='50% CI Leapfrog');

plt.plot(ns, np.mean(times_lf, axis=0)[:], color="blue", label='Median␣
↪Leapfrog')
```

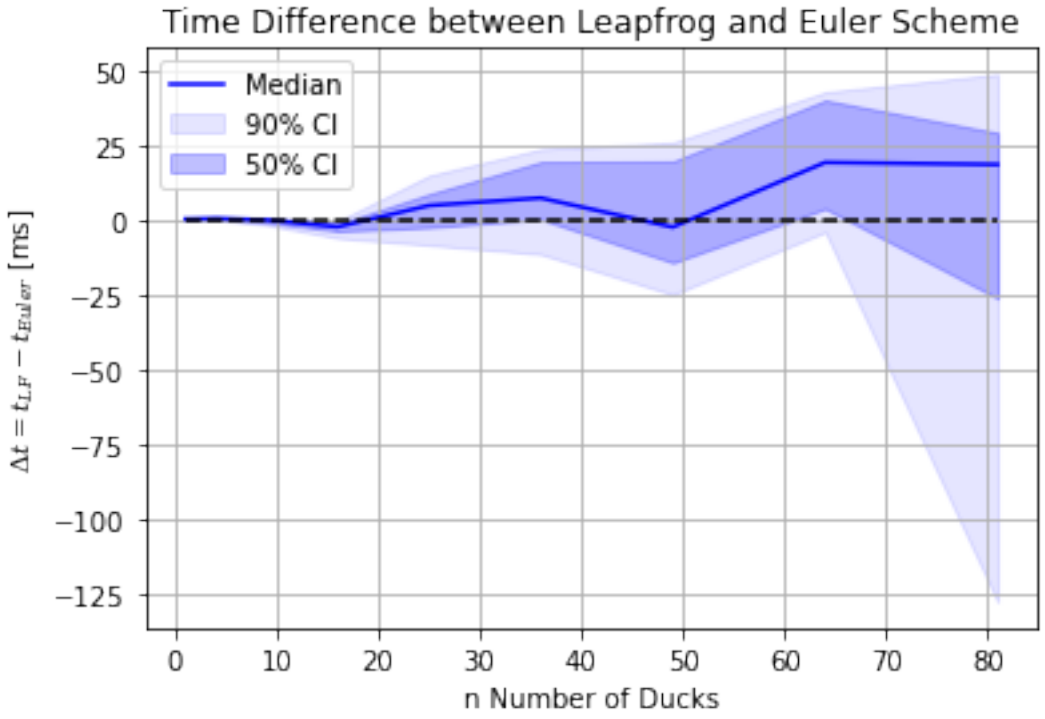
```
plt.fill_between(ns, np.percentile(times_euler, axis=0, q=[10]).ravel()[:],
                     np.percentile(times_euler, axis=0, q=[90]).ravel()[:],
                     alpha = 0.1, color='black', label='90% CI Euler');

plt.fill_between(ns, np.percentile(times_euler, axis=0, q=[25]).ravel()[:],
                     np.percentile(times_euler, axis=0, q=[75]).ravel()[:],
                     alpha = 0.25, color='black', label='50% CI Euler');

plt.plot(ns, np.median(times_euler, axis=0)[:], color="black", label='Median␣
 ↪Euler')

plt.legend()
plt.grid()
plt.xlabel("n Number of Ducks")
plt.ylabel("Execution time t [s]")
plt.title("Execution time for nbody Simulation")
```

[122]:
```
Text(0.5, 1.0, 'Execution time for nbody Simulation')
```



[123]:
```
delta_time = (times_lf-times_euler)*1e3
plt.rcParams["mathtext.fontset"] = "dejavuserif"
plt.plot(ns, np.median(delta_time, axis=0), color="blue", label="Median")
```

```
plt.fill_between(ns, np.percentile(delta_time, axis=0, q=[10]).ravel()[:],
                     np.percentile(delta_time, axis=0, q=[90]).ravel()[:],
                     alpha = 0.1, color='b', label='90% CI');

plt.fill_between(ns, np.percentile(delta_time, axis=0, q=[25]).ravel()[:],
                     np.percentile(delta_time, axis=0, q=[75]).ravel()[:],
                     alpha = 0.25, color='b', label='50% CI');

plt.hlines(0, ns[0], ns[-1], linestyles="--", color="black")

plt.xlabel("n Number of Ducks")
plt.ylabel("$\Delta t=t_{LF}-t_{Euler}$ [ms]")
plt.title("Time Difference between Leapfrog and Euler Scheme")
plt.legend()
plt.grid()
```



Leapfrog is a little big slower than the Euler scheme. The difference is however negligible compared to the overall runtimes of the algorithms.