# Gillespie-Algorithm_Notebook

May 14, 2023

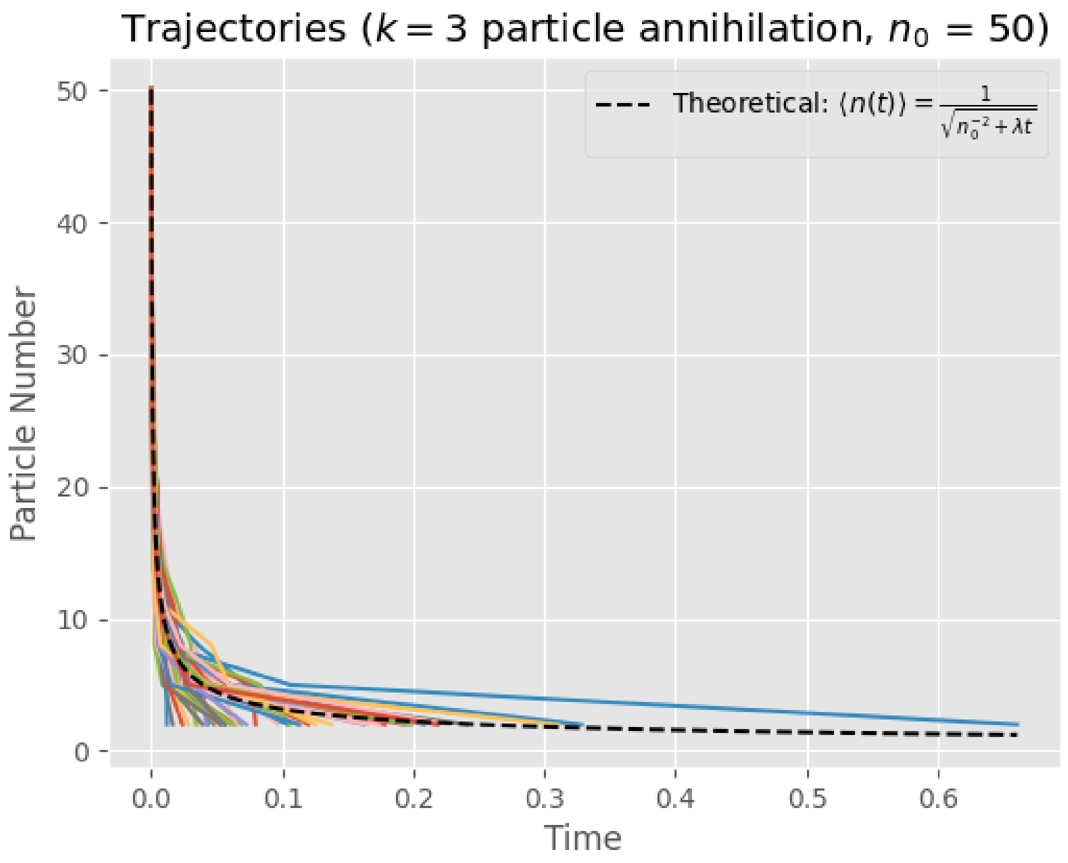
## 1 Open TA: Gillespie algorithm

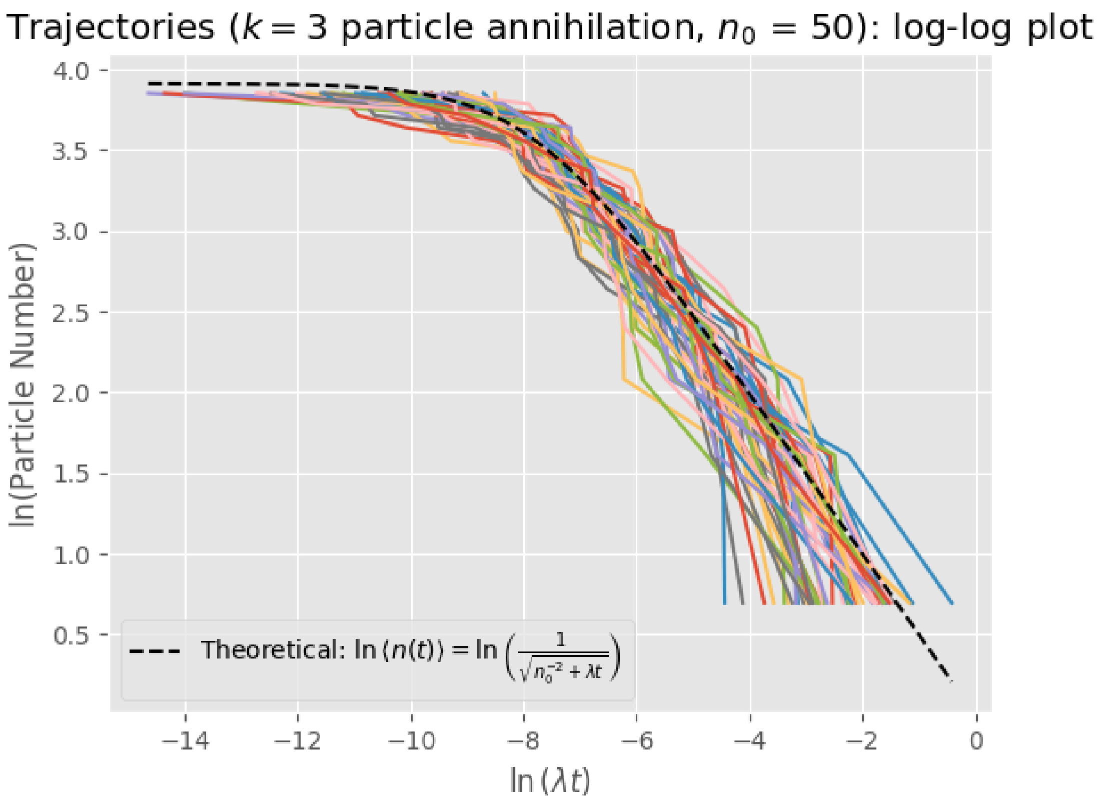
### 1.1 Question d): Implementation

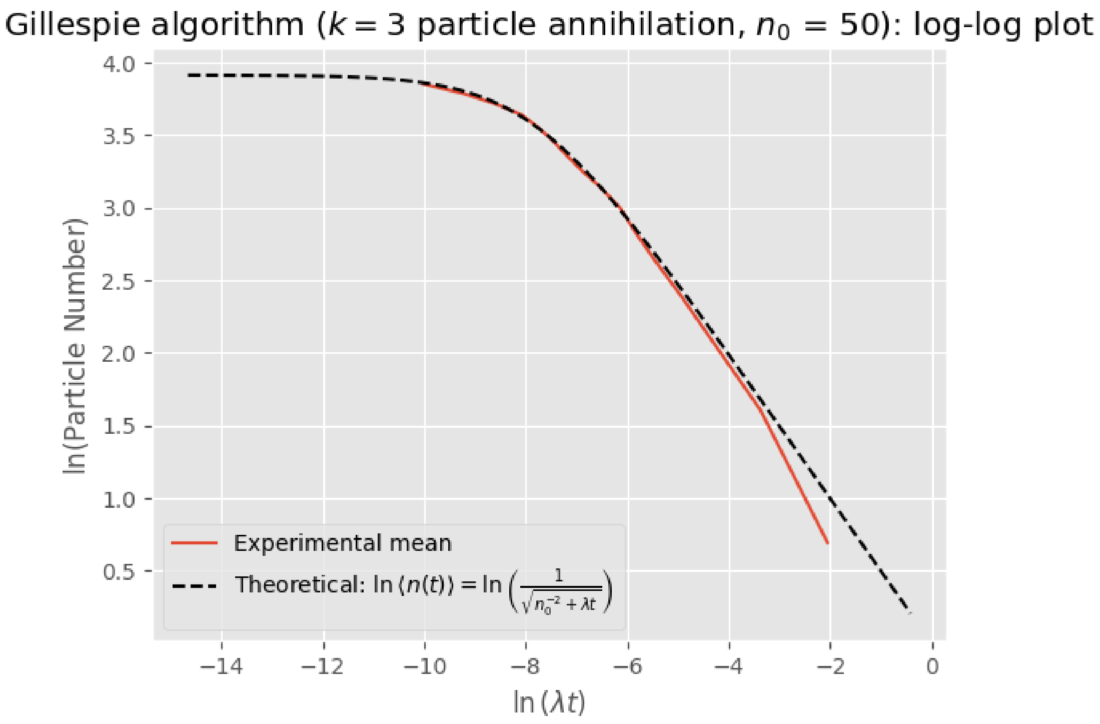
#### 1.1.1 Case A: $n_0 = 50$

[ ]:
```
import random
import matplotlib.pyplot as plt
import numpy as np
import math
plt.style.use('ggplot')

lambda_val = 1.0          # Define the reaction rate constant
n0         = 50; n = n0  # Define the initial particle number
timesVec   = []           # List to store the trajectories
Flag       = True         # Flag
particles = [n0]

for iter in range(50):
    # Define the simulation results
    times = [0.0];
    n     = n0

    # Run the Gillespie algorithm
    while n >= 3:
        # Calculate the reaction probability
        rn = lambda_val * n * (n - 1) * (n - 2) / 6.

        # Draw the next reaction time from an exponential distribution
        tau = -math.log(random.random()) / rn

        # Update the time and particle number
        t = times[-1] + tau
        n -= 3

        # Store the results
        times.append(t)
        if(Flag): particles.append(n)
    timesVec.append(times)
    Flag = False

# Plot the results
for i in range(50):
    plt.plot(timesVec[i], particles)
More_t = np.linspace(min([sorted(tVec)[1] for tVec in timesVec]),␣
  ↪max([max(tVec) for tVec in timesVec]), 1_000_000)
# 'min([sorted(tVec)[1] for tVec in timesVec])': Used to exclude the 0.0 point␣
  ↪in time.
plt.plot(More_t, 1/np.sqrt(n0**(-2) + lambda_val*np.array(More_t)), linestyle =␣
  ↪'dashed',
        label = r'Theoretical: $\left\langlen(t)\right\rangle =␣
  ↪\frac{1}{\sqrt{n_0^{-2} + \lambda t}}$',
        color = 'black', linewidth = 1.5)
plt.xlabel('Time')
plt.ylabel('Particle Number')
plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0})')
plt.legend()
plt.grid(True)
plt.show()

# Plot the results: log-log plot.
for i in range(50): # '[1:]': Needed since we start at t=0. log(0) = -inf,␣
  ↪which is problematic.
    plt.plot(np.log(lambda_val*np.array(timesVec[i])[1:]), np.log(particles)[1:
  ↪])
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
  ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
  ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
  ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
  ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()

# Experimental mean: Awkward definition though.
MeanVec = []
for j in range(len(timesVec[0])):
    MeanVec.append(sum([timesVec[i][j] for i in range(50)])/50.)
```

```
plt.plot(np.log(lambda_val*np.array(MeanVec)[1:]), np.log(particles)[1:], label␣
 ↪= 'Experimental mean')
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
 ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
 ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
 ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Gillespie algorithm ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
 ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()
```



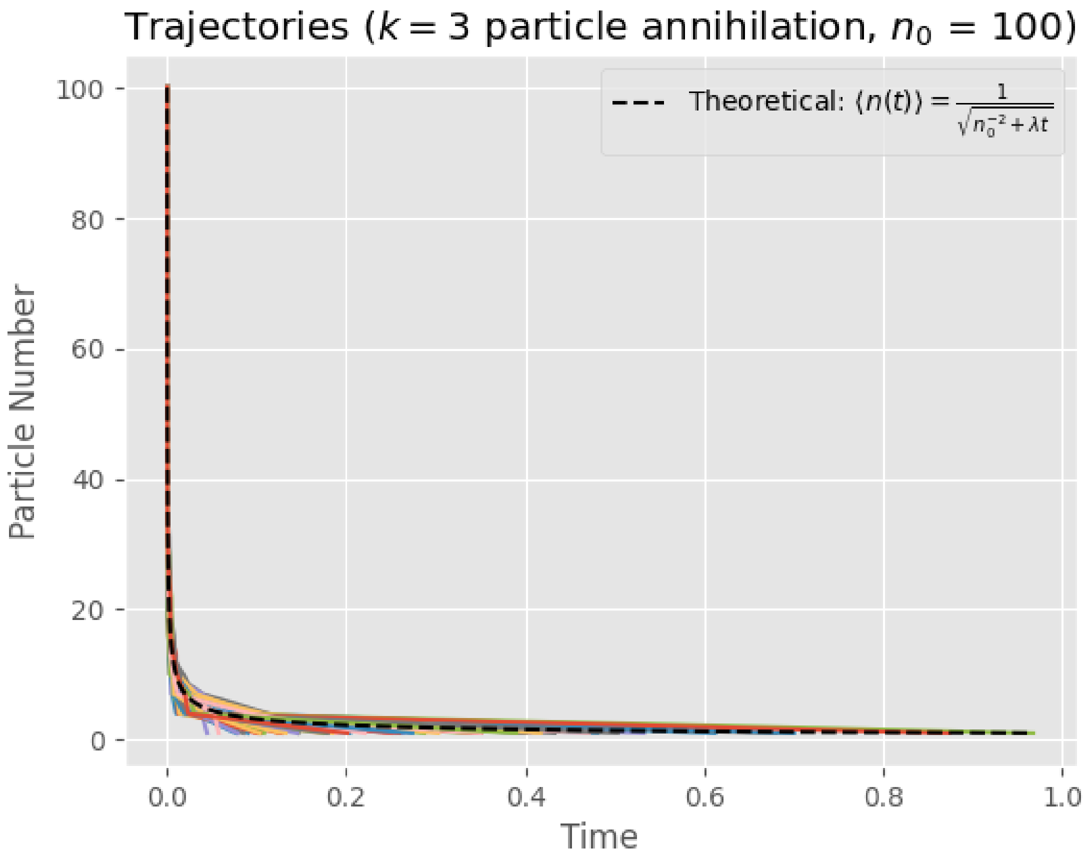

Trajectories ($k = 3$ particle annihilation, $n_0$ = 50): log-log plot
ln(Particle Number)
ln ($\lambda t$)
Theoretical: $\ln \langle n(t) \rangle = \ln \left( \frac{1}{\sqrt{n_0^{-2} + \lambda t}} \right)$
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
−14
−12
−10
−8
−6
−4
−2
0

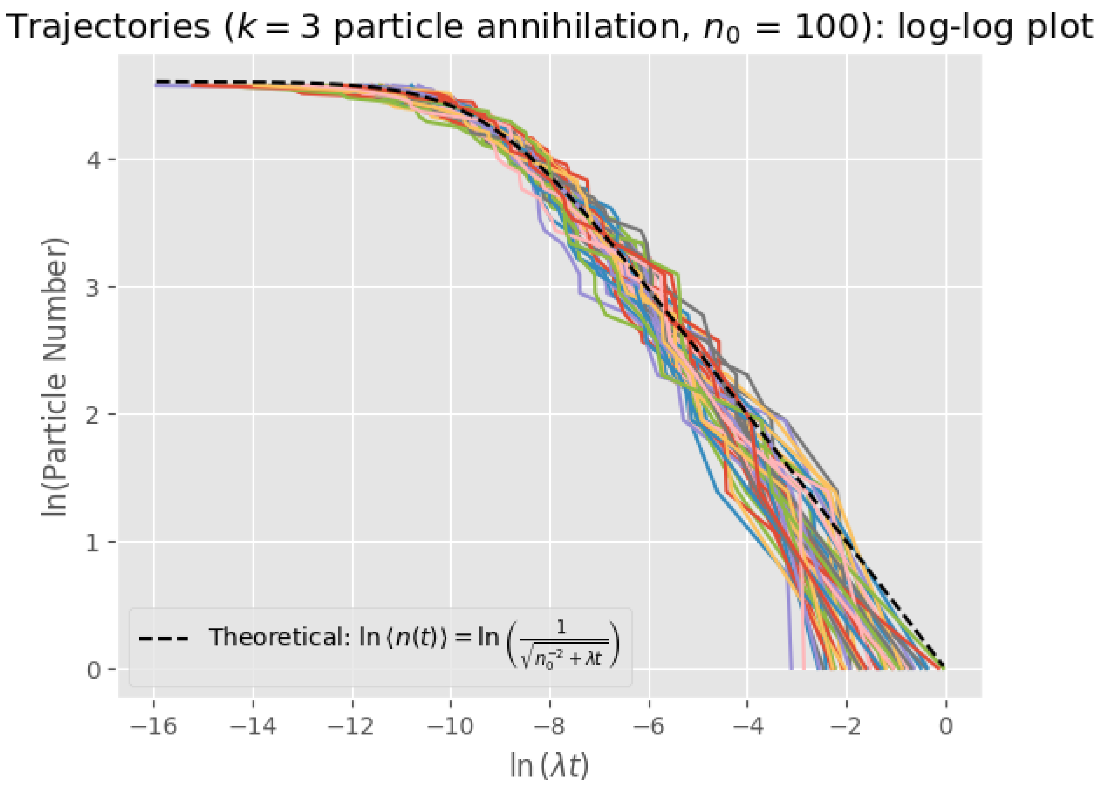

Gillespie algorithm ($k = 3$ particle annihilation, $n_0$ = 50): log-log plot
ln(Particle Number)
ln ($\lambda t$)
Experimental mean
Theoretical: $\ln \langle n(t) \rangle = \ln \left( \frac{1}{\sqrt{n_0^{-2} + \lambda t}} \right)$
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
−14
−12
−10
−8
−6
−4
−2
0

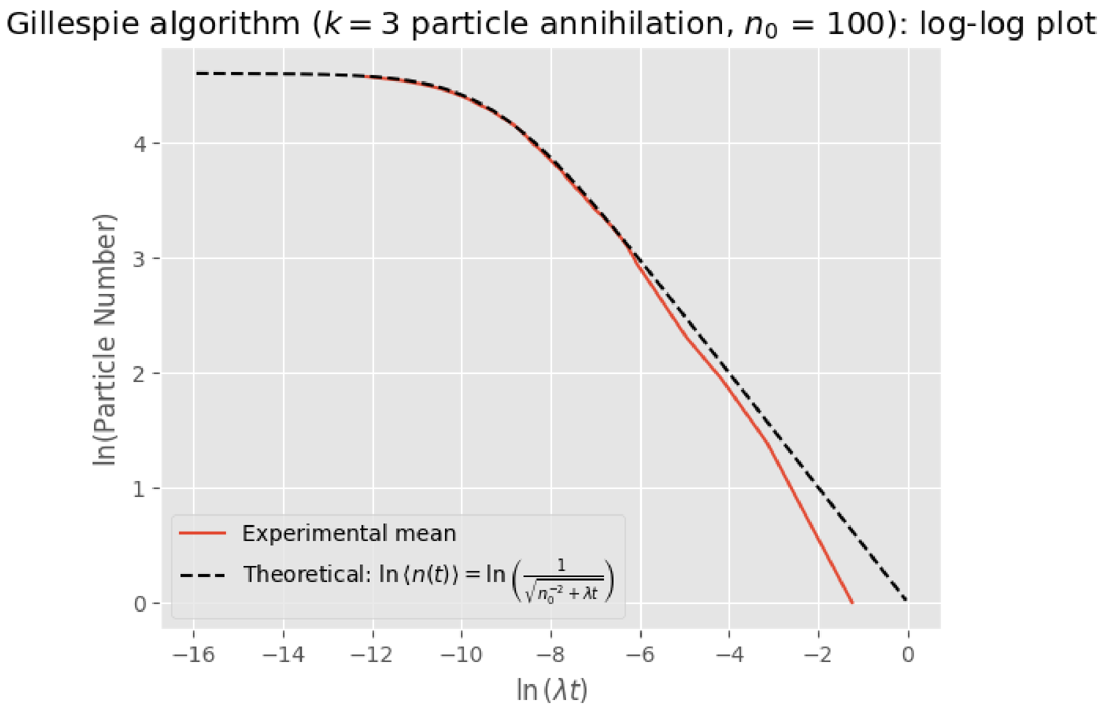
### 1.1.2 Case B: $n_0 = 100$

```
[ ]: lambda_val = 1.0          # Define the reaction rate constant
     n0         = 100; n = n0 # Define the initial particle number
     timesVec   = []          # List to store the trajectories
     Flag       = True        # Flag
     particles = [n0]

     for iter in range(50):
         times = [0.0];
         n     = n0
         while n >= 3:
             rn = lambda_val * n * (n - 1) * (n - 2) / 6.
             tau = -math.log(random.random()) / rn
             t = times[-1] + tau
             n -= 3
             times.append(t)
             if(Flag): particles.append(n)
         timesVec.append(times)
         Flag = False

     # Plot the results
     for i in range(50):
         plt.plot(timesVec[i], particles)
     More_t = np.linspace(min([sorted(tVec)[1] for tVec in timesVec]),␣
      ↪max([max(tVec) for tVec in timesVec]), 1_000_000)
     plt.plot(More_t, 1/np.sqrt(n0**(-2) + lambda_val*np.array(More_t)), linestyle =␣
      ↪'dashed',
             label = r'Theoretical: $\left\langlen(t)\right\rangle =␣
      ↪\frac{1}{\sqrt{n_0^{-2} + \lambda t}}$',
             color = 'black', linewidth = 1.5)
     plt.xlabel('Time')
     plt.ylabel('Particle Number')
     plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0})')
     plt.legend()
     plt.grid(True)
     plt.show()

     # Plot the results: log-log plot.
     for i in range(50): # '[1:]': Needed since we start at t=0. log(0) = -inf,␣
      ↪which is problematic.
         plt.plot(np.log(lambda_val*np.array(timesVec[i])[1:]), np.log(particles)[1:
      ↪])
```

```
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
 ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
 ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
 ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
 ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()

# Experimental mean: Awkward definition though.
MeanVec = []
for j in range(len(timesVec[0])):
    MeanVec.append(sum([timesVec[i][j] for i in range(50)])/50.)

plt.plot(np.log(lambda_val*np.array(MeanVec)[1:]), np.log(particles)[1:], label␣
 ↪= 'Experimental mean')
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
 ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
 ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
 ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Gillespie algorithm ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
 ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()
```

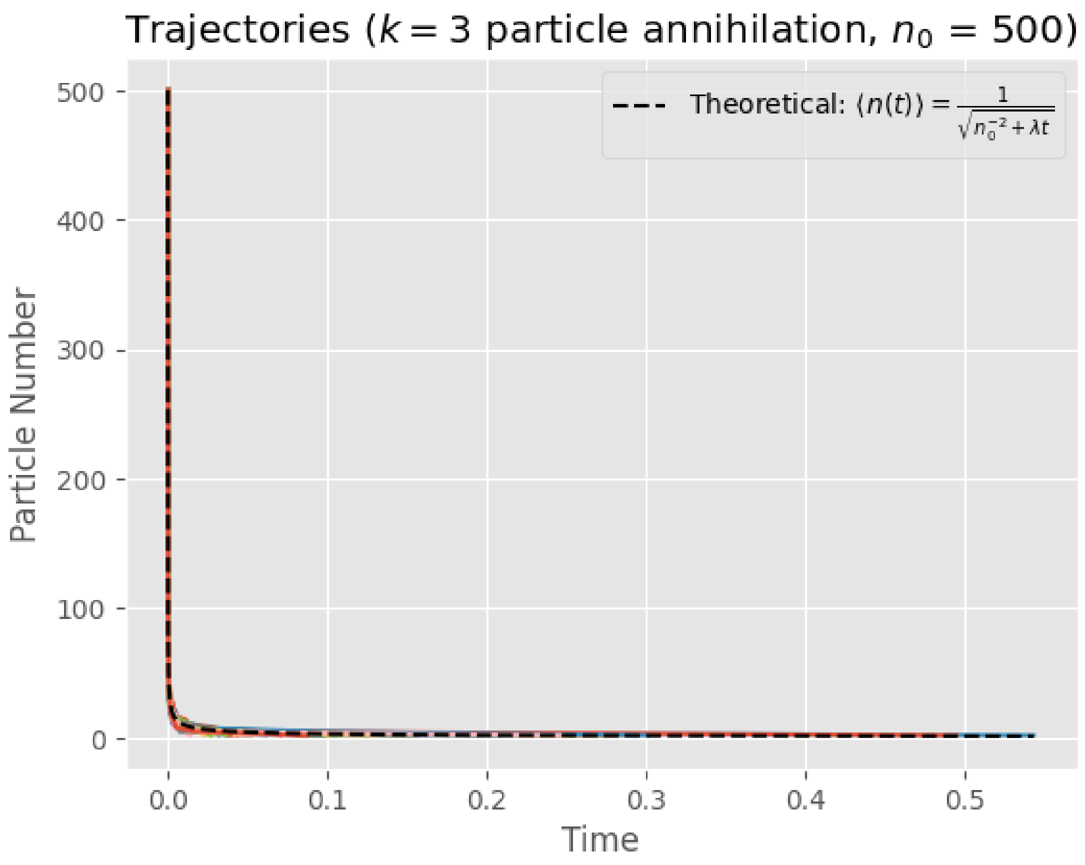

Trajectories ($k = 3$ particle annihilation, $n_0$ = 100)
Theoretical: $\langle n(t) \rangle = \frac{1}{\sqrt{n_0^{-2} + \lambda t}}$
Particle Number
Time
0
20
40
60
80
100
0.0
0.2
0.4
0.6
0.8
1.0

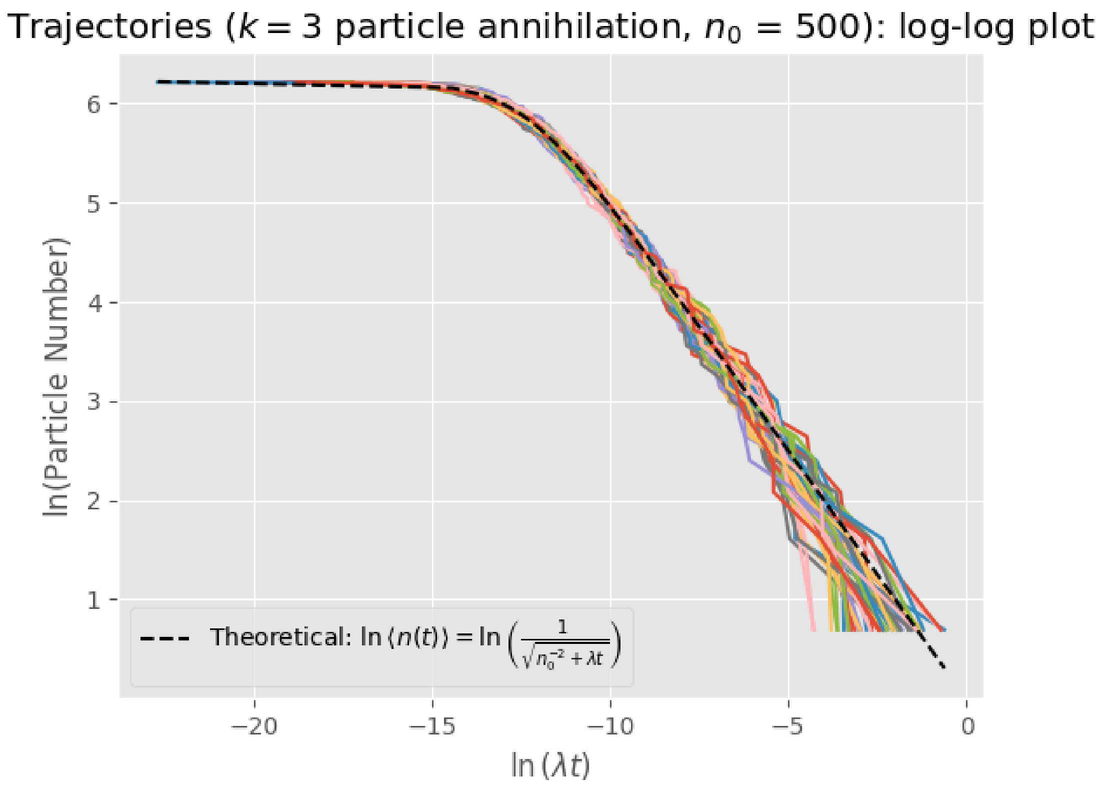

Trajectories ($k = 3$ particle annihilation, $n_0$ = 100): log-log plot
ln(Particle Number)
$\ln(\lambda t)$
Theoretical: $\ln\langle n(t)\rangle = \ln\left(\frac{1}{\sqrt{n_0^{-2}+\lambda t}}\right)$

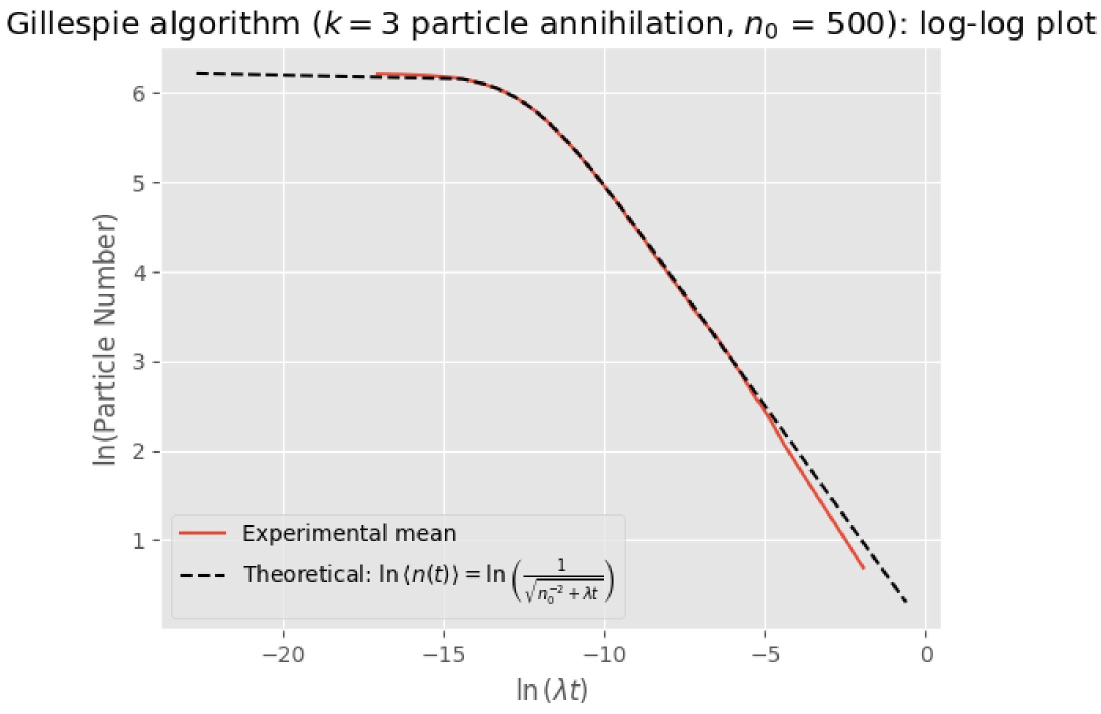

Gillespie algorithm ($k = 3$ particle annihilation, $n_0$ = 100): log-log plot
ln(Particle Number)
$\ln(\lambda t)$
Experimental mean
Theoretical: $\ln\langle n(t)\rangle = \ln\left(\frac{1}{\sqrt{n_0^{-2}+\lambda t}}\right)$

### 1.1.3 Case C: $n_0 = 500$

[ ]:
```
lambda_val = 1.0          # Define the reaction rate constant
n0         = 500; n = n0 # Define the initial particle number
timesVec   = []           # List to store the trajectories
Flag       = True         # Flag
particles = [n0]

for iter in range(50):
    times = [0.0];
    n     = n0
    while n >= 3:
        rn = lambda_val * n * (n - 1) * (n - 2) / 6.
        tau = -math.log(random.random()) / rn
        t = times[-1] + tau
        n -= 3
        times.append(t)
        if(Flag): particles.append(n)
    timesVec.append(times)
    Flag = False

# Plot the results
for i in range(50):
    plt.plot(timesVec[i], particles)
More_t = np.linspace(min([sorted(tVec)[1] for tVec in timesVec]),␣
 ↪max([max(tVec) for tVec in timesVec]), 1_000_000)
plt.plot(More_t, 1/np.sqrt(n0**(-2) + lambda_val*np.array(More_t)), linestyle =␣
 ↪'dashed',
        label = r'Theoretical: $\left\langlen(t)\right\rangle =␣
 ↪\frac{1}{\sqrt{n_0^{-2} + \lambda t}}$',
        color = 'black', linewidth = 1.5)
plt.xlabel('Time')
plt.ylabel('Particle Number')
plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0})')
plt.legend()
plt.grid(True)
plt.show()

# Plot the results: log-log plot.
for i in range(50): # '[1:]': Needed since we start at t=0. log(0) = -inf,␣
 ↪which is problematic.
    plt.plot(np.log(lambda_val*np.array(timesVec[i])[1:]), np.log(particles)[1:
 ↪])
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
 ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
  ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
  ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Trajectories ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
  ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()

# Experimental mean: Awkward definition though.
MeanVec = []
for j in range(len(timesVec[0])):
    MeanVec.append(sum([timesVec[i][j] for i in range(50)])/50.)

plt.plot(np.log(lambda_val*np.array(MeanVec)[1:]), np.log(particles)[1:], label␣
  ↪= 'Experimental mean')
plt.plot(np.log(lambda_val*np.array(More_t)), np.log(1/np.sqrt(n0**(-2) +␣
  ↪lambda_val*np.array(More_t))), linestyle = 'dashed',
    label = r'Theoretical: $\ln{\left\langlen(t)\right\rangle} =␣
  ↪\ln{\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)}$',
    color = 'black', linewidth = 1.5) # Fix  this graph. It starts mid-way␣
  ↪through.
plt.xlabel('$\ln{(\lambda t)}$')
plt.ylabel(r'$\ln($Particle Number$)$')
plt.title(rf'Gillespie algorithm ($k = 3$ particle annihilation, $n_0$ = {n0}):␣
  ↪log-log plot')
plt.legend()
plt.grid(True)
plt.show()
```


Trajectories ($k = 3$ particle annihilation, $n_0$ = 500)
Theoretical: $\langle n(t) \rangle = \frac{1}{\sqrt{n_0^{-2} + \lambda t}}$
Particle Number
Time
0
100
200
300
400
500
0.0
0.1
0.2
0.3
0.4
0.5


Trajectories ($k = 3$ particle annihilation, $n_0 = 500$): log-log plot
ln(Particle Number)
ln $(\lambda t)$
Theoretical: $\ln\langle n(t)\rangle = \ln\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)$


Gillespie algorithm ($k = 3$ particle annihilation, $n_0 = 500$): log-log plot
ln(Particle Number)
ln $(\lambda t)$
Experimental mean
Theoretical: $\ln\langle n(t)\rangle = \ln\left(\frac{1}{\sqrt{n_0^{-2} + \lambda t}}\right)$

The results appear to be more accurate when $n_0$ is bigger. This is consistent with our assumption that $\langle n(t) \rangle \gg 1$. This is a lot more apparent in the initial part of the trajectory, for small $t$, where $n(t)$ is still large. In this region, the agreement with the theoretical prediction is clearly sharper. As $n(t)$ goes down, our approximation becomes less and less accurate, which explains the deviation of the experimental results from the theoretical prediction.