

Collaborators

I worked with **Andrew Binder**, and **Adarsh Iyer** to complete this homework.

Schroeder 2.5 (5 pts)

For an Einstein solid with each of the following values of N and q , list all of the possible microstates, count them, and verify formula 2.9.

- a) $N = 3, q = 4$

Solution: Here we'll just generate a table and show out all the microstates, just like how it's done in the book:

Oscillator	#1	#2	#3
	1	1	2
	1	2	1
2	1	1	1
	1	0	3
	1	3	0
0	1	3	
	0	3	1
3	1	0	
	3	0	1
4	0	0	
	0	4	0
0	0	4	
2	2	0	0
2	0	2	
0	2	2	

In total there are 15 different configurations. Plugging it into the formula, we get:

$$\Omega(3, 4) = \binom{3+4-1}{4} = \binom{6}{4} = 15$$

as desired. □

- d) $N = 4, q = 2$

Solution: Just like the previous problem, we generate a table:

Oscillator	#1	#2	#3	#4
0	0	1	1	
0	1	0	1	
1	0	0	1	
0	1	1	0	
1	0	1	0	
1	1	0	0	
0	0	0	2	
0	0	2	0	
0	2	0	0	
2	0	0	0	

So there are 10 possible configurations. Again, using formula 2.9:

$$\Omega(4, 2) = \binom{4+2-1}{2} = \binom{5}{2} = 10$$

as desired. □

f) $N = 1, q = \text{anything}$

Solution: Since $N = 1$, then whatever q is, all those units of energy must go into the single particle that we have, so $\Omega = 1$ in this case. Using formula 2.9:

$$\Omega(1, q) = \binom{1+q-1}{q} = \binom{q}{q} = 1$$

□

g) $N = \text{anything}, q = 1$

Solution: Since we only have one energy packet and there are N different particles, then there are consequently N different ways we can choose where to give this “energy packet,” hence this gives us $\Omega = N$.

This is also confirmed by the formula

$$\Omega(N, 1) = \binom{1+N-1}{1} = \binom{N}{1} = N$$

□

Schroeder 2.8 (5 pts)

Consider a system of two Einstein solids, A and B , each containing 10 oscillators, sharing a total of 20 units of energy. Assume that the solids are weakly coupled, and that the total energy is fixed.

- a) How many different *macrostates* are available to this system?

Solution: The macrostate is defined as the amount of energy in A and amount of energy in B . There are 21 possible configurations, since the minimum amount of energy in one of the Einstein solids (which automatically determines the energy in the other) is 0 units, and the maximum is 20 units. \square

-
- b) How many different *microstates* are available to this system?

Solution: We use formula 2.9, where $N = 20$ and $q = 20$:

$$\Omega(20, 20) = \binom{39}{20} = 6.89 \times 10^{10}$$

\square

- c) Assuming that this system is in thermal equilibrium, what is the probability of finding all the energy in solid A ?

Solution: There is only one configuration in which all the energy is in solid A , so the probability is $\frac{\Omega(10,20)}{\Omega(\text{all})} = 1.45 \times 10^{-4}$. \square

- d) What is the probability of finding exactly half of the energy in solid A ?

Solution: We need to calculate the number of microstates where exactly 10 units of energy are found within solid A and also within solid B . This means that we can treat solids A and B as independent, and multiply the two counts together. Then, we divide by the total number of microstates to finally get our probability. Thus:

$$\Omega(AB) = \frac{\binom{19}{10} \binom{19}{10}}{\binom{39}{20}} \approx 12\%$$

\square

- e) Under what circumstances would this system exhibit irreversible behavior?

Solution: This system would exhibit irreversible behavior whenever we let it move toward thermal equilibrium, or in other words let the system settle into its most likely state. \square

Schroeder 2.18 (10 pts)

Use Stirling's approximation to show that the multiplicity of an Einstein solid, for any large values of N and q , is approximately

$$\Omega(N, q) \approx \frac{\left(\frac{q+N}{q}\right)^q \left(\frac{q+N}{N}\right)^N}{\sqrt{2\pi q(q+N)/N}}$$

The square root in the denominator is merely large, and can often be neglected. However, it is needed in Problem 2.22. (Hint: First show that $\Omega = \frac{N}{q+N} \frac{(q+N)!}{q!N!}$. Do not neglect the $\sqrt{2\pi N}$ in Stirling's approximation.

Solution: First, we do the hint:

$$\Omega(N, q) = \binom{N+q-1}{q} = \frac{(N+q-1)!}{q!(N-1)!} = \frac{N}{N+q} \frac{(N+q)!}{q!N!}$$

Now, we apply Sterling's formula in the form $x! = x^x e^{-x} \sqrt{2\pi x}$:

$$\begin{aligned} \Omega(N, q) &\approx \frac{N}{N+q} \frac{(N+q)^{N+q} e^{-(N+q)} \sqrt{2\pi(N+q)}}{q^q e^{-q} \sqrt{2\pi q} \cdot N^N e^{-N} \sqrt{2\pi N}} \\ &= \frac{N}{N+q} \frac{(N+q)^{N+q}}{N^N q^q} \cdot \sqrt{\frac{N+q}{2\pi N q}} \\ &= \frac{\left(\frac{N+q}{N}\right)^N \left(\frac{N+q}{q}\right)^q}{\sqrt{\frac{2\pi N q}{(N+q)} \cdot \frac{(N+q)^2}{N^2}}} \\ &= \frac{\left(\frac{N+q}{N}\right)^N \left(\frac{N+q}{N}\right)^q}{\sqrt{2\pi q(N+q)/N}} \end{aligned}$$

Sorry if I'm not showing *every* single step of algebra, if I did then this simplification would take way too long. \square

Ising Ferromagnet (15 pts)

Consider a system of N -magnetic moments each of which takes binary values $\sigma_i = \pm 1$ with $i = 1, 2, \dots, N$. So there are $\Omega(\text{all}) = 2^N$ microstates, just like the 2-state model. The energy, however, takes the form of a *ferromagnet*

$$E = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}$$

Note that the first and last spin talk only with the spin to their right/left respectively (the geometry is a finite-length chain.)

- a) What are the very lowest energy microstates of the ferromagnet, and what are their energy? (We call these the ground states.) What do the microstates look like with an energy just above them?

Solution: To create the lowest energy state, we want $\sigma_i \sigma_{i+1} = 1$, this can happen in two different ways: either $\sigma_i = \sigma_{i+1} = 1$ or $\sigma_i = \sigma_{i+1} = -1$. Therefore, the lowest energy microstate is one where all the magnetic moments are aligned with one another. Here, since all $\sigma_i = \pm 1$, then this means that this state has an energy $E = -J(N - 1)$. Visually this is:

$$\overbrace{\uparrow \dots \uparrow \dots \uparrow}^N$$

To generate the next energy, notice that when two consecutive σ_i are equal, it actually doesn't matter whether they're spin up or spin down - they contribute the same amount to the final summation. Therefore, the only time we will increase the energy in the system when we have the case where $\sigma_i = -\sigma_{i+1}$ or vice versa.

Consider the case where there are "domains of moments," where we have a chain of moments that are of all aligned with one another. This contributes the smallest amount of energy gain, since it introduces only one pair of moments which are anti-aligned. Therefore, the energy state just above them is the state where we have two domains of moments, or alternatively one invisible "wall" between them. Visually, this looks like:

$$\uparrow \dots \uparrow | \downarrow \dots \downarrow$$

where the vertical line here denotes our "wall" where the spins flip. This contributes the lowest energy gain, and hence it is the energy just above the ground state. \square

- b) Derive an expression for the total number of microstates $\Omega(N, q)$ where $E = -J(N - 1) + J2q$. Hint: there is a clever trick you can apply here which maps the problem almost exactly to one we solved in class!

Solution: We know that $E = -J(N - 1)$ is the ground state energy, so therefore we need to introduce $2Jq$ energy into the system. Notice that when we introduce a wall, we add $2J$ units of energy, since we change that particular product of $\sigma_i \sigma_{i+1}$ from $-J$ to J . Therefore, we require q walls to generate $2Jq$ energy.

Effectively, this means our problem becomes finding the number of ways of distributing q walls among N items, which is exactly the stars and bars problem. Therefore, the number of ways is:

$$\Omega(N, q) = \binom{N-1}{q}$$

Finally, consider the fact that if we flip *all* the spins, it doesn't change the energy (since the summation doesn't prefer spin up over spin down), so for every configuration we count, there's a corresponding one with all the spins flipped. Therefore, the total number actually is:

$$\Omega(N, q) = 2 \binom{N-1}{q}$$

\square

State Counting (20 pts)

I would like to conduct numerical experiments of the ideal gas, but it is a bit tricky because you have to solve $F = ma$ for colliding particles. So, in the spirit of the “spherical cow”, in this problem you will develop an approximate treatment of a gas by breaking up space into a discrete grid.

For simplicity, we will assume our particles move only in the 2D x - y plane. We discretize space into a square grid of small boxes each of volume Δr^2 , labeled by their centers (x, y) . Now here is where we make a simplification: rather than keeping track of the *exact* location of each particle, we will only keep track of the number of particles in each box, $n(x, y) = 0, 1, 2, \dots$. The microstate of the system is then labeled by the collection of integers $\{n(x, y)\}$ where $\sum_{x,y} n(x, y) = N$ is the total number of particles.

- a) Explain why $\{n(x, y)\}$ is sufficient to recover the precise location of all the particles if we take $\Delta r^2 \rightarrow 0$ while holding the average particle density fixed. (You may wonder about permutations of the particles ... we'll come back to this when we discuss the Gibbs Paradox)

Solution: Consider the case where we have a particle in our particular grid. Our uncertainty in the position of that particle comes directly from the size of the square, since we can't say anything about where inside the square the particle resides. Therefore, if we reduce the size of the square (i.e. $\Delta r \rightarrow 0$), then we are reducing our uncertainty in the location of all particles, meaning that by just shrinking Δr it is indeed sufficient to recover the precise location. \square

Henceforth, we'll choose units such that $\Delta r^2 = 1$ for notational simplicity. There are $V = L_x \cdot L_y$ such boxes labeled by integer pairs (x, y) .

- b) Suppose the energy is entirely independent of $\{n(x, y)\}$, is an ideal gas without a gravitational potential. How many microstates $\Omega(V, N)$ are there for a system with V -boxes and N particles? Hint: you already know the answer!

Solution: There's N particles that we have to place into V boxes, this is the same problem as having N units of energy, and we need to place it into V oscillators. Therefore, the number of microstates is:

$$\Omega(V, N) = \binom{V + N - 1}{N}$$

\square

- c) Consider an $V = L_x \times L_y = 20 \times 20$ system which we partition into $V_A = 9 \times 20$ region and a $V_B = 11 \times 20$ region, with $N = N_A + N_B = 100$ particles. Following the fundamental assumption of statistical mechanics (and assuming particles are never created or destroyed), obtain a mathematical expression for the probability $P(N_A)$ to observe N_A particles in region A. Evaluate $P(N_A = 40)$ using e.g. Mathematica.

Solution: First note that we have the following expression for $P(N_A)$:

$$P(N_A) = \frac{\Omega(V_A, N_A)\Omega(V_B, N_B)}{\Omega(\text{all})}$$

We have 100 particles and $V = 400$, so $\Omega(\text{all}) = \Omega(400, 100)$. Then, the volume of region A is $V_A = 180$, $V_B = 220$. Therefore, we have:

$$P(N_A) = \frac{\binom{V_A+N_A-1}{N_A}\binom{V_B+N_B-1}{N_B}}{\binom{V+N-1}{N}} = \frac{\binom{180+40-1}{40}\binom{220+60-1}{60}}{\binom{400+100-1}{100}} \approx 0.048$$

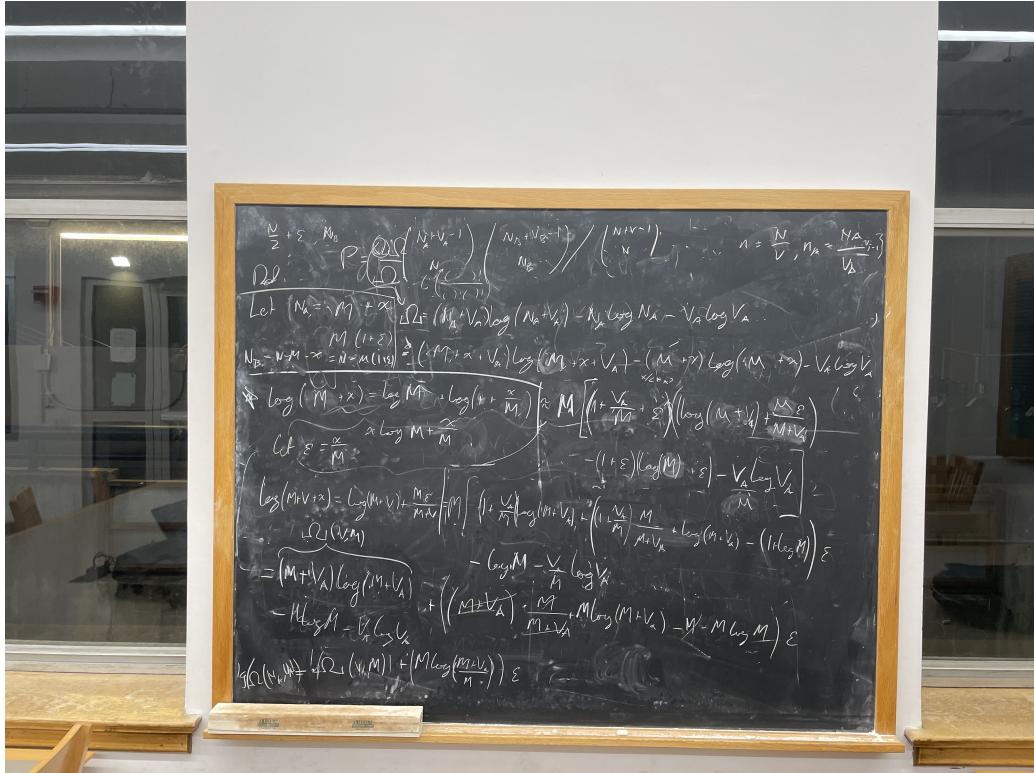
\square

- d) Use Stirling's approximation in the form $\ln x! = x \ln x - x$ to approximately bring $P(\langle N_A \rangle)$ to the form $P(N_A) = P(N_A)e^{-\frac{1}{2}(N_A - \langle N_A \rangle)^2/\sigma^2}$. What is the average $\langle N_A \rangle$ and standard deviation $\sigma = \sqrt{\langle (N_A - \langle N_A \rangle)^2 \rangle}$ for the parameters of Part 2? Hint: your answer will take a fairly nice form if expressed in terms of V , $\frac{V_A}{V_B}$, $n = \frac{N}{V}$, $n_A = \frac{N_A}{V_A}$. If you'd like to use Mathematica at some point that's fine (I did): just be explicit in what step it was used for.

Solution: So this problem was incredibly annoying, myself and a couple friends spent a very long time and basically got nowhere with the expression. We first simplified the expression using Stirling's formula by hand, and we got the following equations:

$$\begin{aligned}\ln \Omega(V_A, N_A) &= \ln \Omega(V_A, \langle N_A \rangle) + \epsilon \langle N_A \rangle \ln \left(\frac{\langle N_A \rangle + V_A}{\langle N_A \rangle} \right) \\ \ln \Omega(V_B, N_B) &= \ln \Omega(V_B, N - \langle N_A \rangle) - \epsilon M \ln \left(\frac{N - \langle N_A \rangle + V_B}{N - \langle N_A \rangle} \right) \\ \ln \Omega(V, N) &= (N + V) \ln(1 + n) - N \log n\end{aligned}$$

where we've defined $\epsilon = \frac{x}{\langle N_A \rangle}$, $x = N_A - \langle N_A \rangle$ and $n = \frac{N}{V}$. Below are the photos of my work:



In fond memory of endless chats and talks - Michael Doyen (79) and Thomas Reinhardt-Marques (79)

$$\begin{aligned}
 N_A &= \langle N_A \rangle + x = M + x \\
 \log \Omega(M, N_A) &= \log(\Omega(N_A, M) + M \log \frac{N_A}{M}) \varepsilon \\
 \log \Omega(N_A, N_B) &= \log(\Omega(N_B, N_A) + N_B \log \frac{N_A}{N_B}) \varepsilon \\
 \log \Omega(N_A, N_B) &= (N_A + V_B) \log(M + V_A) - H_B \log N_B \\
 &\quad - (N_A - x) \log(N_A - M - x) - V_B \log V_B \\
 &\quad + (N_A - x) \log(V_A) + (N_A - x) \log(N_A - M - x) - V_B \log V_B \\
 &\quad + M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \frac{M}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A}{M} \right) \right) \right] \\
 &= M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \frac{M}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A}{M} \right) \right) \right] - \frac{M}{M} (1-\varepsilon) V_B \\
 &= M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \left(\frac{M}{M} (1-\varepsilon) \log M + \log \left(\frac{N_A}{M} \right) \right) \right] - \frac{M}{M} (1-\varepsilon) V_B \\
 &= M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \left(\frac{M}{M} (1-\varepsilon) \log M + \log \left(\frac{N_A}{M} \right) \right) \right] - M \log \frac{M+V_B}{M} \varepsilon \\
 &= M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \left(\frac{M}{M} (1-\varepsilon) \log M + \log \left(\frac{N_A}{M} \right) \right) \right] - M \log \frac{M+V_B}{M} \varepsilon \\
 &= M \left[\frac{M+V_B}{M} (1-\varepsilon) \left(\log M + \log \left(\frac{N_A+V_B}{M} \right) \right) - \left(\frac{M}{M} (1-\varepsilon) \log M + \log \left(\frac{N_A}{M} \right) \right) \right] - M \log \frac{M+V_B}{M} \varepsilon
 \end{aligned}$$

$$\begin{aligned}
 & (N_A + V_B) \log(M + V_A) - M \log N_A - V \log V = \log(\Omega(M, N_A)) \\
 n = \frac{M}{V} & \rightarrow V \left[(1+n) (\log V + \log(1+n)) - n \log n V - \log V \right] \\
 & = V \left[\log V + n \log V + \log(1+n) + n \log(1+n) - n \log n V - \log V \right] \\
 & = V \left[n \log V + \log(1+n) (1+n) - n \log n V \right] \\
 & = V \left[n \log V + (1+n) \log(1+n) - n \log n - n \log V \right] \\
 & = V \left[(1+n) \log(1+n) - n \log n \right] \\
 & = (M+V) \log(1+n) - M \log n
 \end{aligned}$$

I didn't want to type out all the algebra since it would be a lot, but in essence, we expanded $N_A = \langle N_A \rangle + x$ where x is some small quantity, then performed the Taylor expansion of $\ln(1+x)$ around $x = 0$ wherever possible. We also used the suggested expressions of $n = \frac{N}{V}$ and $n_A = \frac{N_A}{V_A}$. We then simplified this further by using the initial expression for $\Omega(V, N)$, but this ultimately didn't get us down to the desired form. \square

-
- e) We have approximated the gas' microstates by $\{n(x, y)\}$. As $\Delta r^2 \rightarrow 0$, do you think this gives a reasonable counting of all the microstates of a mono-atomic ideal gas? Or are we missing degrees of freedom? Explain.

Solution: This does not give a reasonable counting, since $\{n(x, y)\}$ only gives information about the *position* of the particles, but not its momentum. Since we're missing these degrees of freedom in our calculations, this is not an accurate counting of all the microstates. \square

Problem 6: Numerical Simulation (20 pts)

I couldn't find a good way to attach the file, so I downloaded my python code by converting it to a PDF and attached it below. However, due to the way that the code blocks render, the formula doesn't wrap, but instead just goes off the page, so for some lines only half of the code in that line is visible. Unfortunately there isn't an easy fix for this, but if there's a way please do let me know so I can do it for future submissions.

Problem 6: Numerical Simulation

Importing necessary libraries; I chose to use the random package instead of the random generator provided by numpy, though I think numpy calls on `random.randint()` to execute its calculation anyway so it doesn't make much of a difference.

In [1]:

```
import numpy as np
import random

import matplotlib.pyplot as plt
```

In [2]:

```
initial = np.zeros((20, 20)) # makes initial array

#populates initial array with 100 particles
for _ in range(100):
    col = random.randint(0, 8)
    row = random.randint(0, 19)

    initial[row, col] += 1

short = np.copy(initial)
long = np.copy(initial)

# function used to simulate the array
def simulate(array, t) -> list:

    n_A = []
    for i in range(0, t):
        col = random.randint(0, 19)
        row = random.randint(0, 19)
        if array[row, col] > 0:
            new_row = random.randint(-1, 1)
            new_col = random.randint(-1, 1)

            array[row, col] -= 1
            array[(row + new_row)%20, (col + new_col)%20] += 1 # place particle

        #count the stuff
        n_A.append(np.sum(array[:,0:9]))

    return n_A

n_short = simulate(short, 10000) #plotting for part (a)
n_long = simulate(long, 2 * 10**6)
```

The cell below just makes a bunch of plots. For part (a), we wanted to plot what it looked like after a few iterations - I chose this value to be $n = 10000$ since I found that any smaller n almost made it seem like there wasn't any movement at all. Here, we can see that a good fraction of the particles have made it into V_B , but the majority of particles are still found in V_A . However, we can see that after 2×10^6 steps, the gas really has distributed itself out such that the distribution looks pretty uniform.

In [3]:

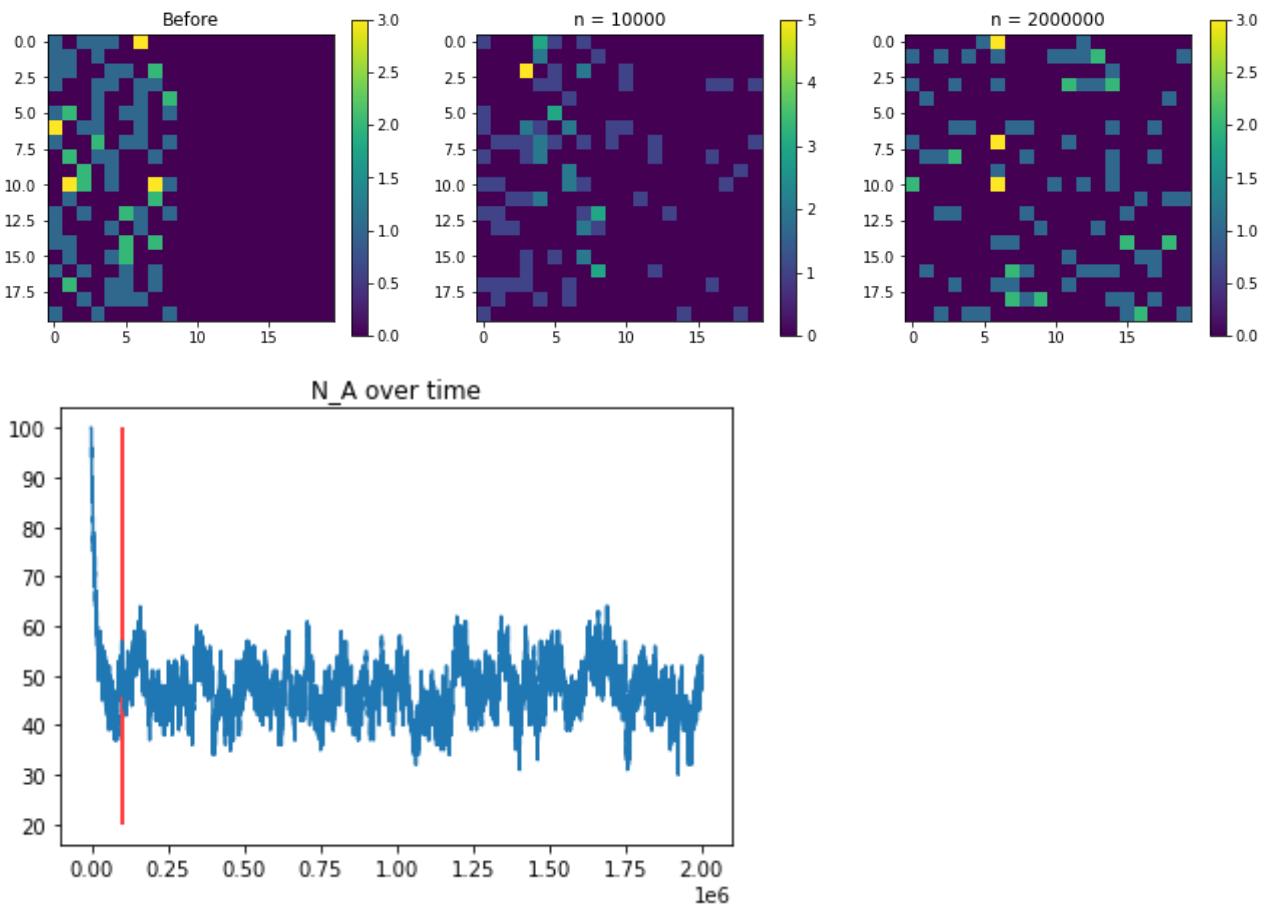
```
# cell for plots
fig, axs = plt.subplots(1, 3)
fig.set_figwidth(15)

plot = axs[0].imshow(initial)
fig.colorbar(plot, ax = axs[0])
axs[0].set_title("Before")

plot2 = axs[1].imshow(short)
fig.colorbar(plot2, ax = axs[1])
axs[1].set_title("n = 10000")

plot3 = axs[2].imshow(long)
fig.colorbar(plot3, ax = axs[2])
axs[2].set_title("n = 2000000")
plt.show()

fig2 = plt.plot(n_long)
plt.vlines(100000, 20, 100, color = 'red')
plt.title("N_A over time")
plt.show()
```



Here I hard-coded the fact that we'll take $t_{eq} = 100000$ since it seems to be a reasonable threshold when I ran my simulations (I didn't pick a smaller t_{eq} since I wanted a guarantee that we've reached equilibrium). Therefore, the mean and standard deviation will be computed with the array `n_long[100000:]`.

In [4]:

```

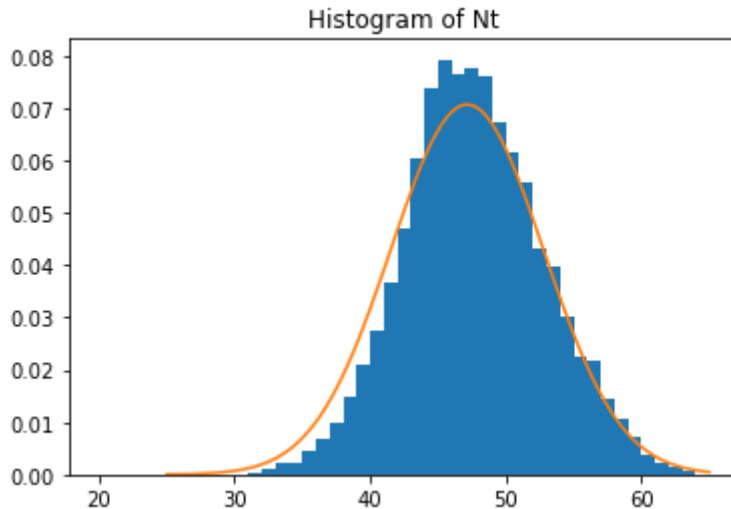
sigma = np.std(n_long[1000000:])
mu = np.mean(n_long[1000000:])
# mu = (100/400) * 100

fig3 = plt.hist(n_long[100000:], density=True, bins=np.arange(20, 65, 1))

x_values = np.linspace(25, 65, 100)
y_values = 1/np.sqrt(2*np.pi*sigma**2) * np.exp(-1/2 * (x_values - mu)**2/sigma**2)

plt.plot(x_values, y_values)
plt.title("Histogram of Nt")
plt.show()

```



Unfortunately, since I didn't get a clean expression for problem 5d, there's really no way for me to proceed further with the actual comparison step (I used the statistics to plot the bell curve, so obviously it fits very well). That said, we can calculate what the mean and standard deviation *should* be from a statistical argument, with the assumption that the particles are evenly distributed. Using this assumption, the expression for the mean is:

$$N_A = \frac{N \cdot V_A}{V} = \frac{(100)(180)}{400} \approx 45$$

This expression is obtained by assuming that every "box" has equal density, so we just multiply that by V_A to get N_A . I expect that this is the expected result from 5d as well, but unfortunately I cannot confirm that. Further, we also expect that the standard deviation follows the following form:

$$\sigma = \sqrt{\langle (N_A - \langle N_A \rangle)^2 \rangle}$$

This expression comes straight from the problem statement of 5d. Computing these values in the cell below:

In [5]:

```

print(f"Mean of N_A (data): {np.mean(n_long[100000:])} \n")

print(f"Standard deviation of N_A (data): {sigma}")
print(f"Standard deviation of N_A (formula) {np.sqrt(np.mean((n_long[100000:] - 

```

```
Mean of N_A (data): 47.15079052631579
```

```
Standard deviation of N_A (data): 5.641484570492062
Standard deviation of N_A (formula) 5.118341642030339
```

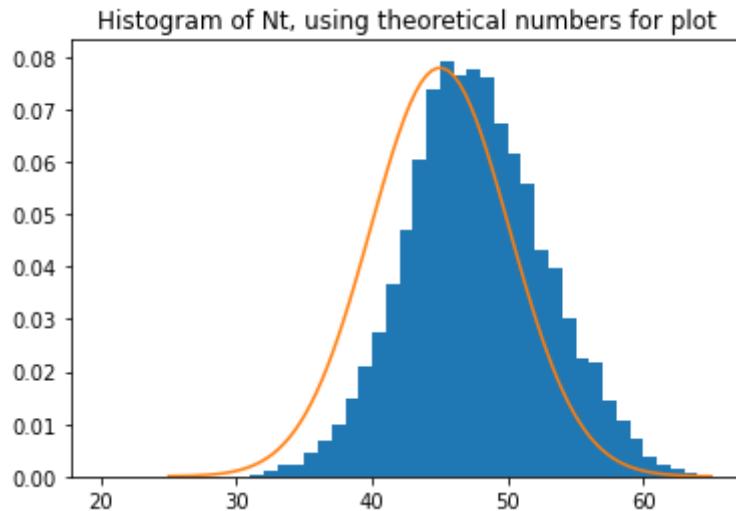
Firstly, we see that the mean of N_A from the simulated data matches up almost perfectly with our expected mean from our statistical argument. Further, our standard deviation from the simulated data matches very well with the expected standard deviation of a normal distribution. This result, combined with the gaussian curve (orange) in the histogram provides strong evidence that our N_A indeed follows a Gaussian distribution exactly as we expected, and our numbers match perfectly.

That said, the value for the standard deviation is slightly off from what we expect, but also not too far that it can't just be statistical error. Finally, as another demonstration of the fact that these values indeed do work:

In [6]:

```
mu_theory = 45
std_theory = np.sqrt(np.mean((n_long[100000:] - mu)**2))

fig3 = plt.hist(n_long[100000:], density=True, bins=np.arange(20, 65, 1))
x_values = np.linspace(25, 65, 100)
y_values = 1/np.sqrt(2*np.pi*std_theory**2) * np.exp(-1/2 * (x_values - mu_theory)**2)
plt.plot(x_values, y_values)
plt.title("Histogram of Nt, using theoretical numbers for plot")
plt.show()
```



As expected, when we use the theoretical values for $\langle N_A \rangle$ and σ , the curve still fits our data very well, therefore confirming that our distribution is indeed Gaussian.