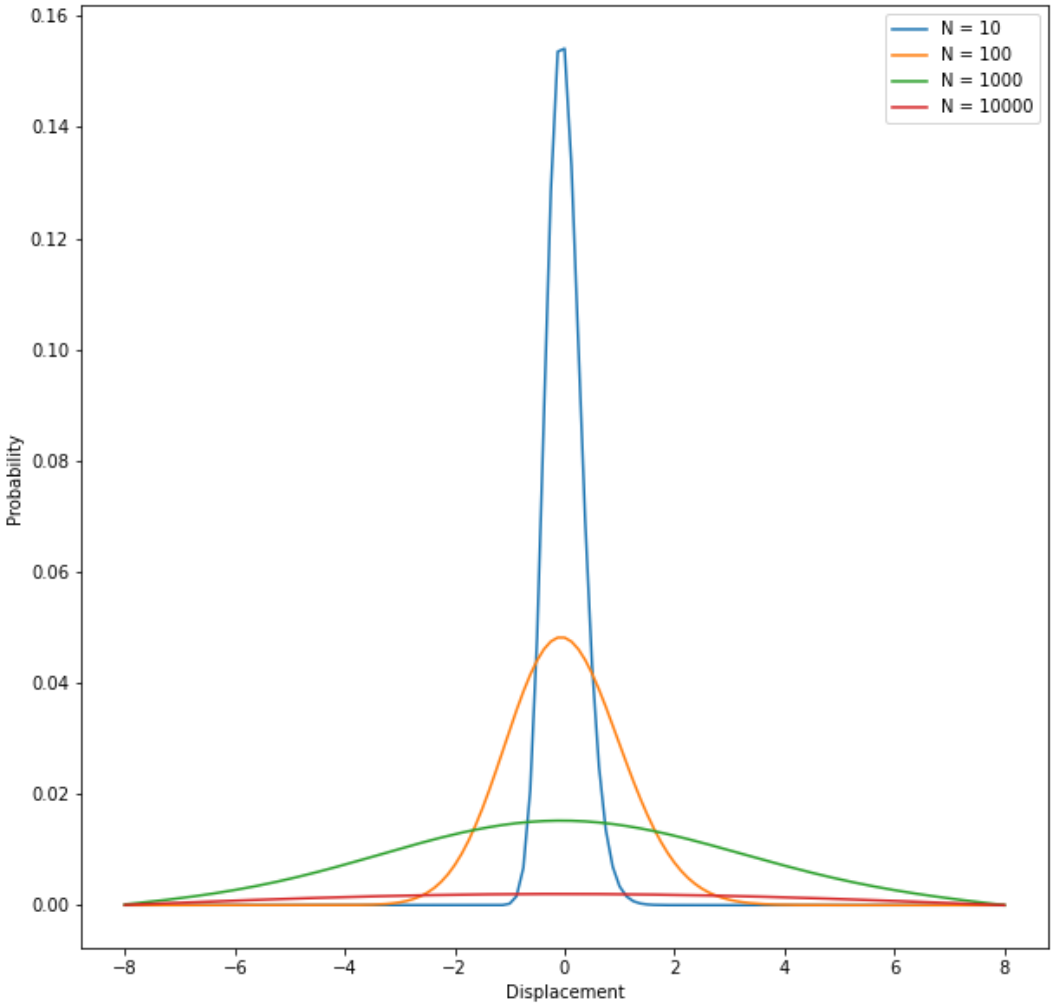
Question 4

1D Diffusion

The graphs for 1D Diffusion at timestamps T=10, 100, 1000 and 10,000 is as follows:



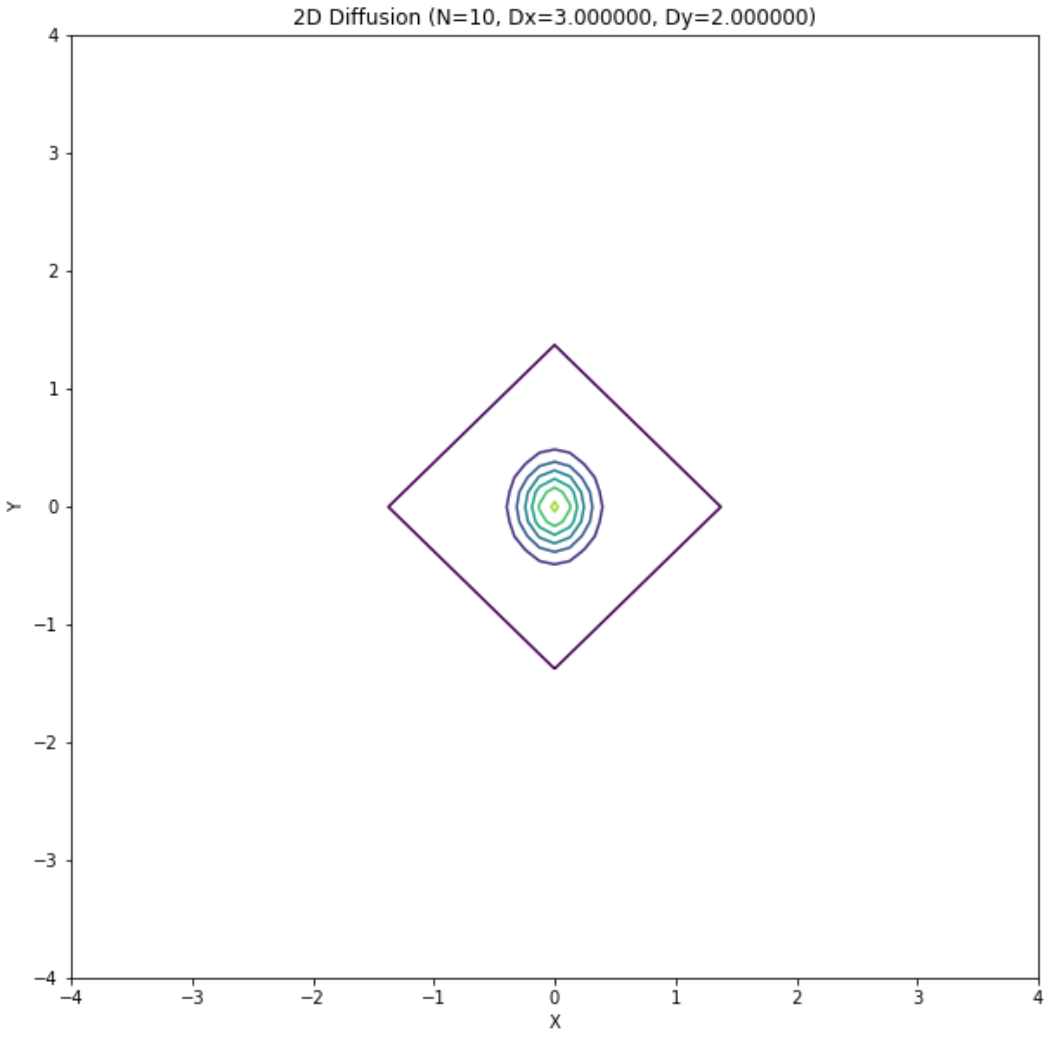
As time progresses, the probability of the molecule being found at its initial position decreases and that of being found at the near boundary increases. This is expected as the gas diffuses.

2D Diffusion

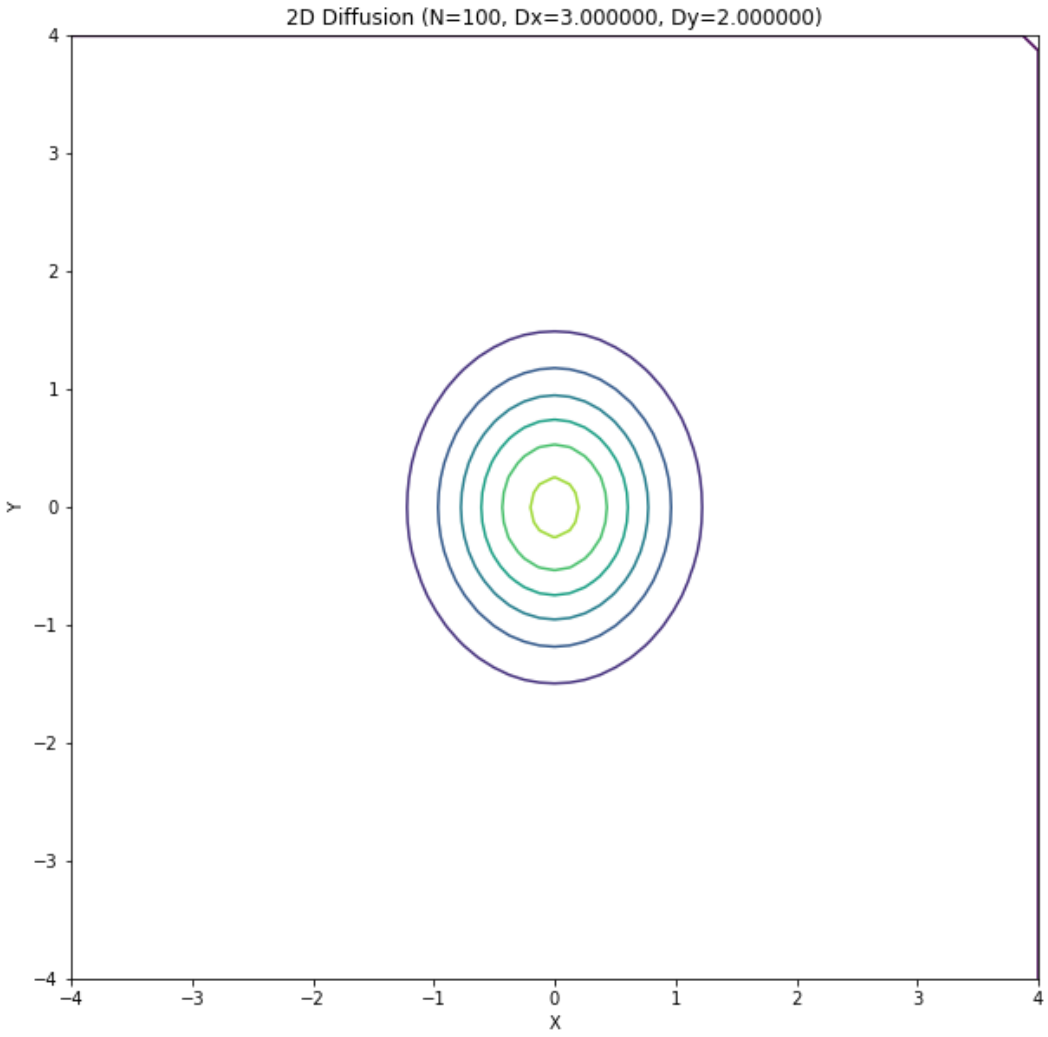
The contour plots of probabilities at different time values and different cases are as follows:

Case 1 : Dx > Dy:

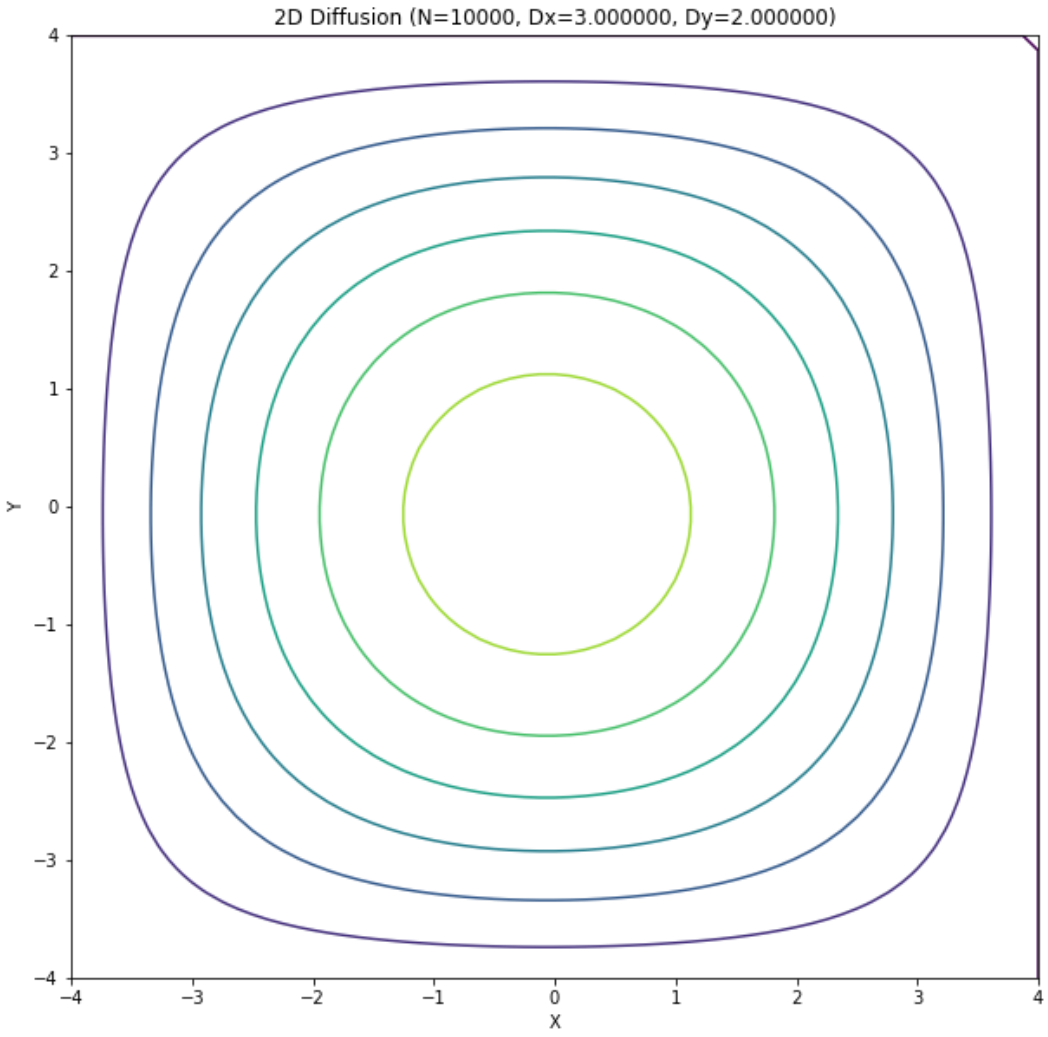
N = 10


2D Diffusion (N=10, Dx=3.000000, Dy=2.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

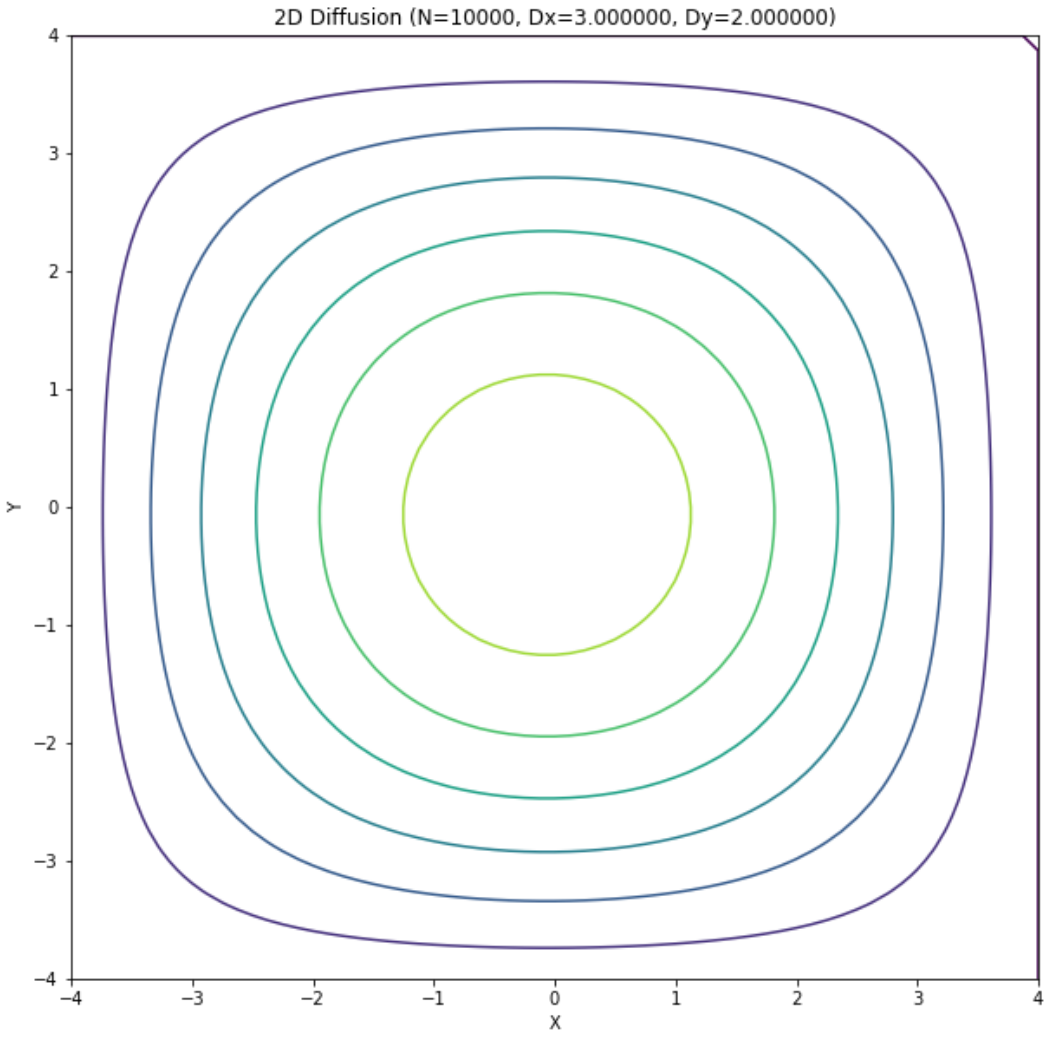
N = 100


2D Diffusion (N=100, Dx=3.000000, Dy=2.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 1000

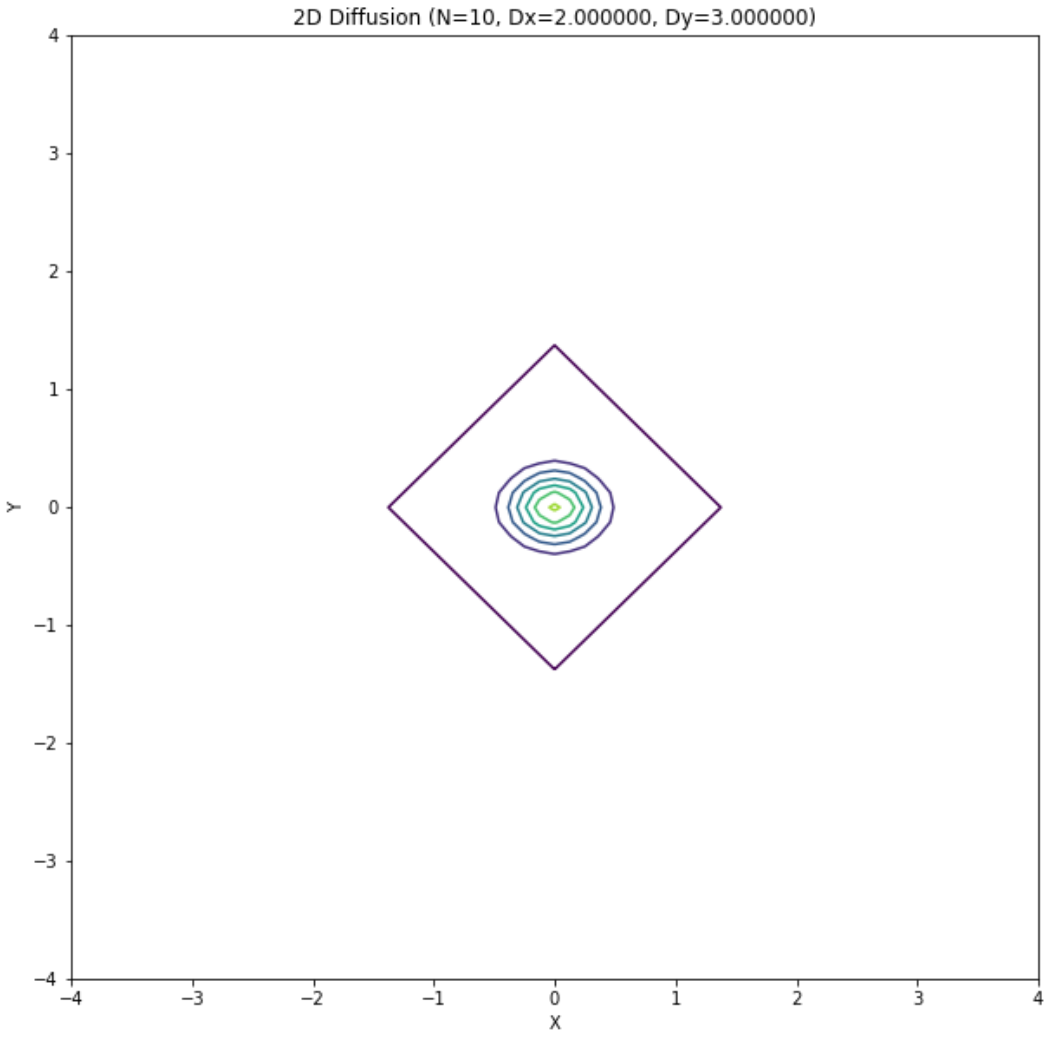

2D Diffusion (N=10000, Dx=3.000000, Dy=2.000000)
X
Y
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 10000

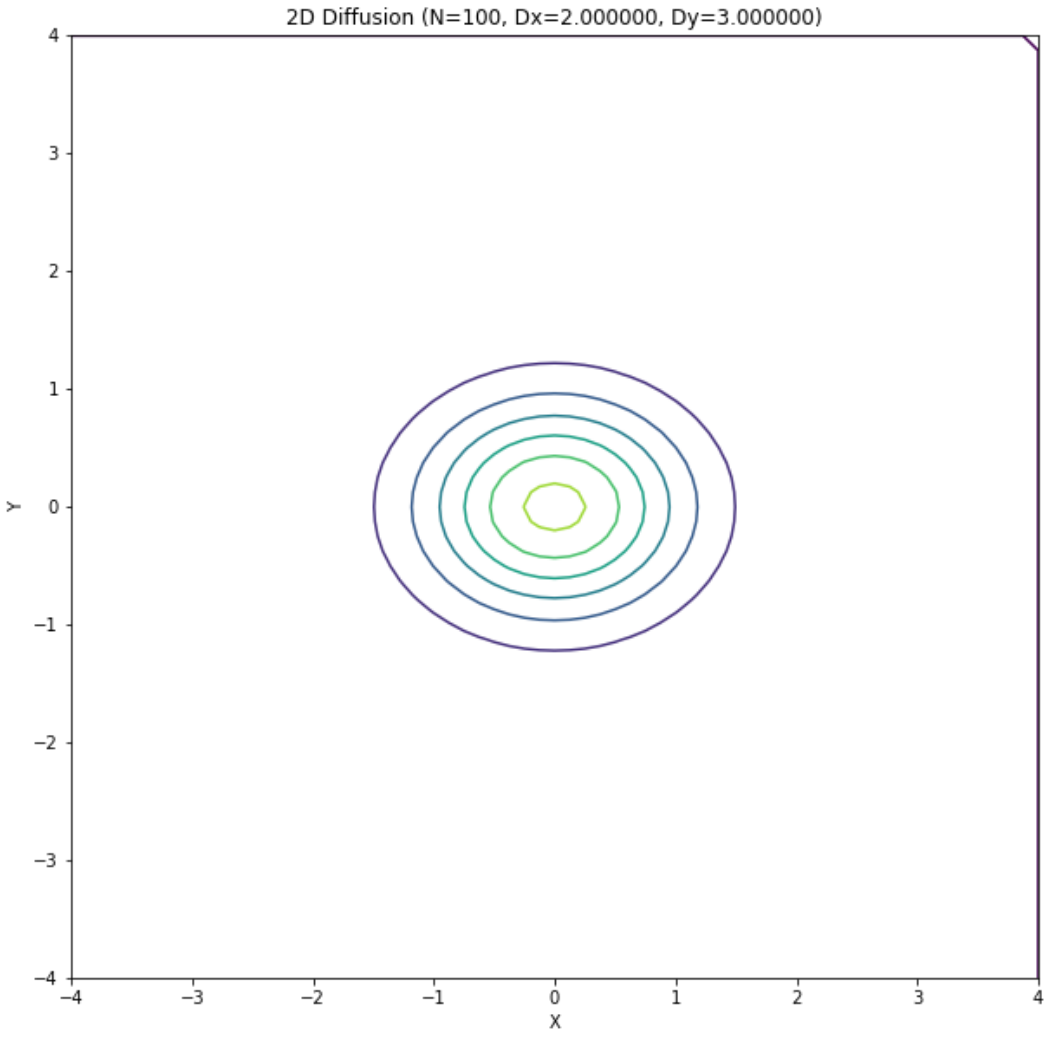


Case 2: Dx < Dy

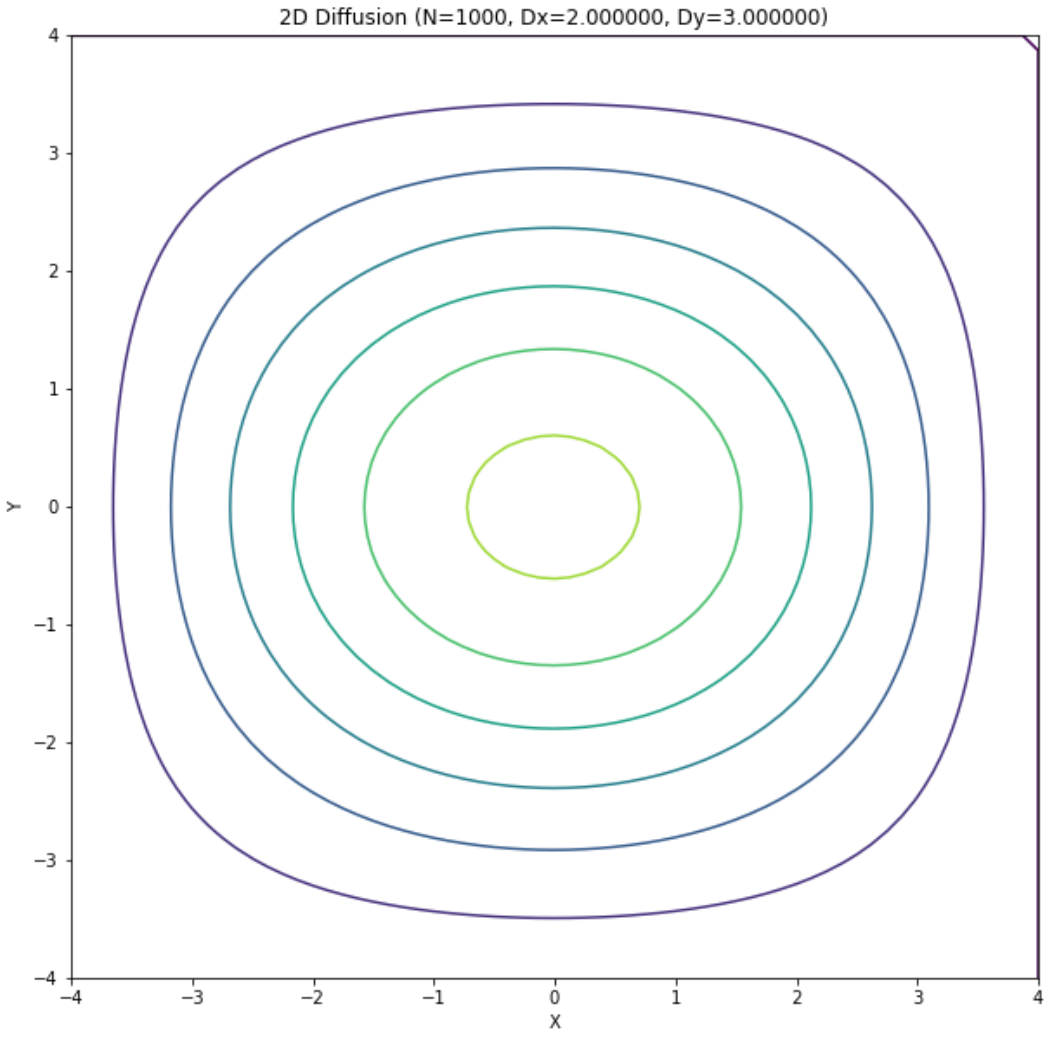
N = 10


2D Diffusion (N=10, Dx=2.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

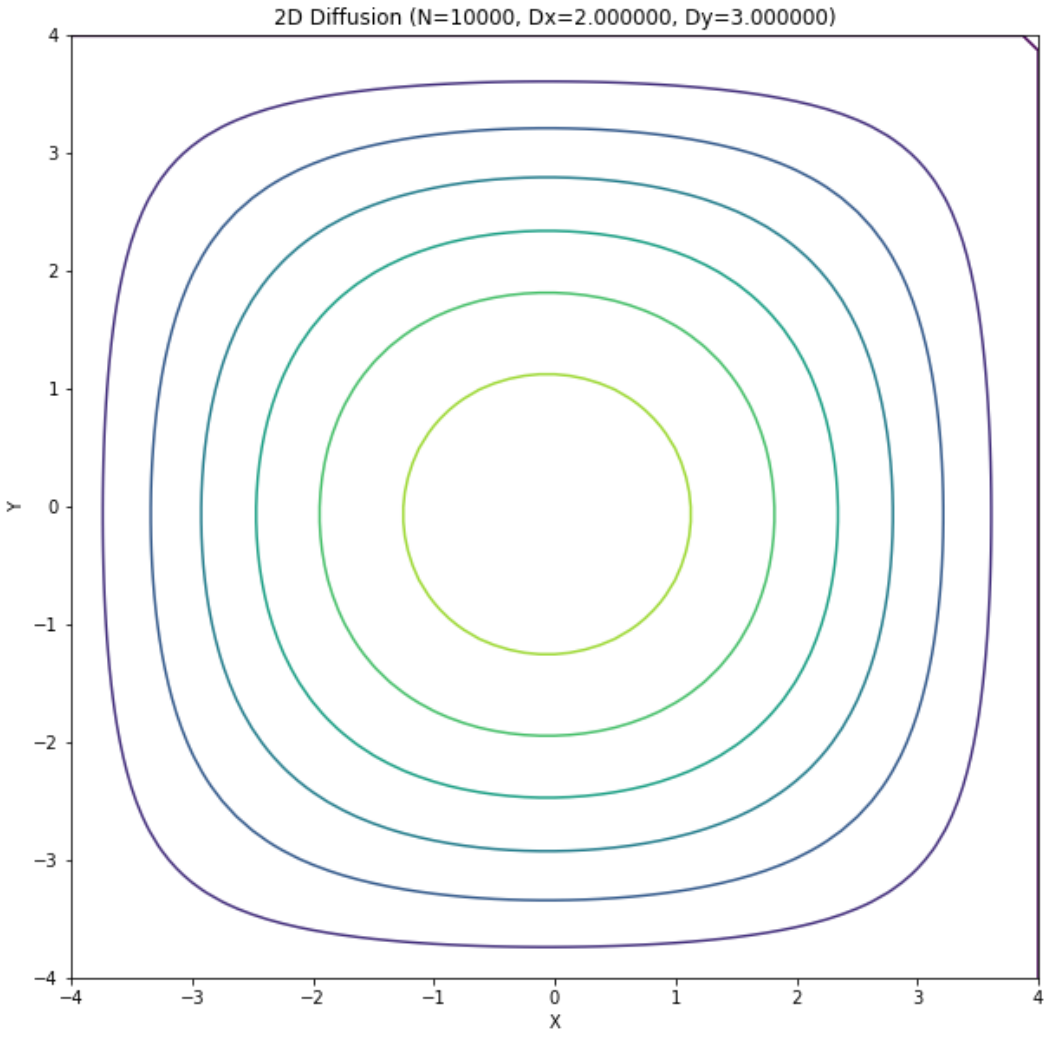
N = 100


2D Diffusion (N=100, Dx=2.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 1000

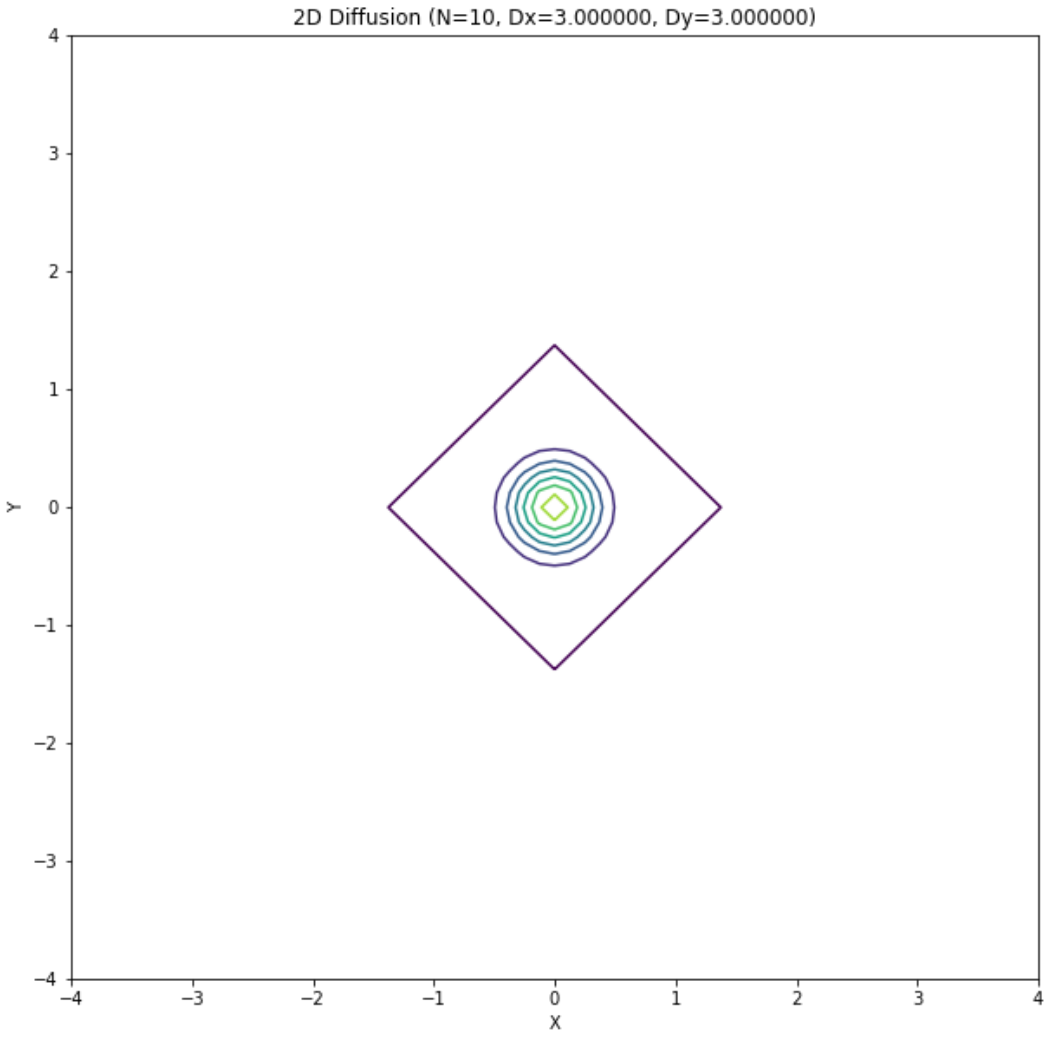

2D Diffusion (N=1000, Dx=2.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 10000

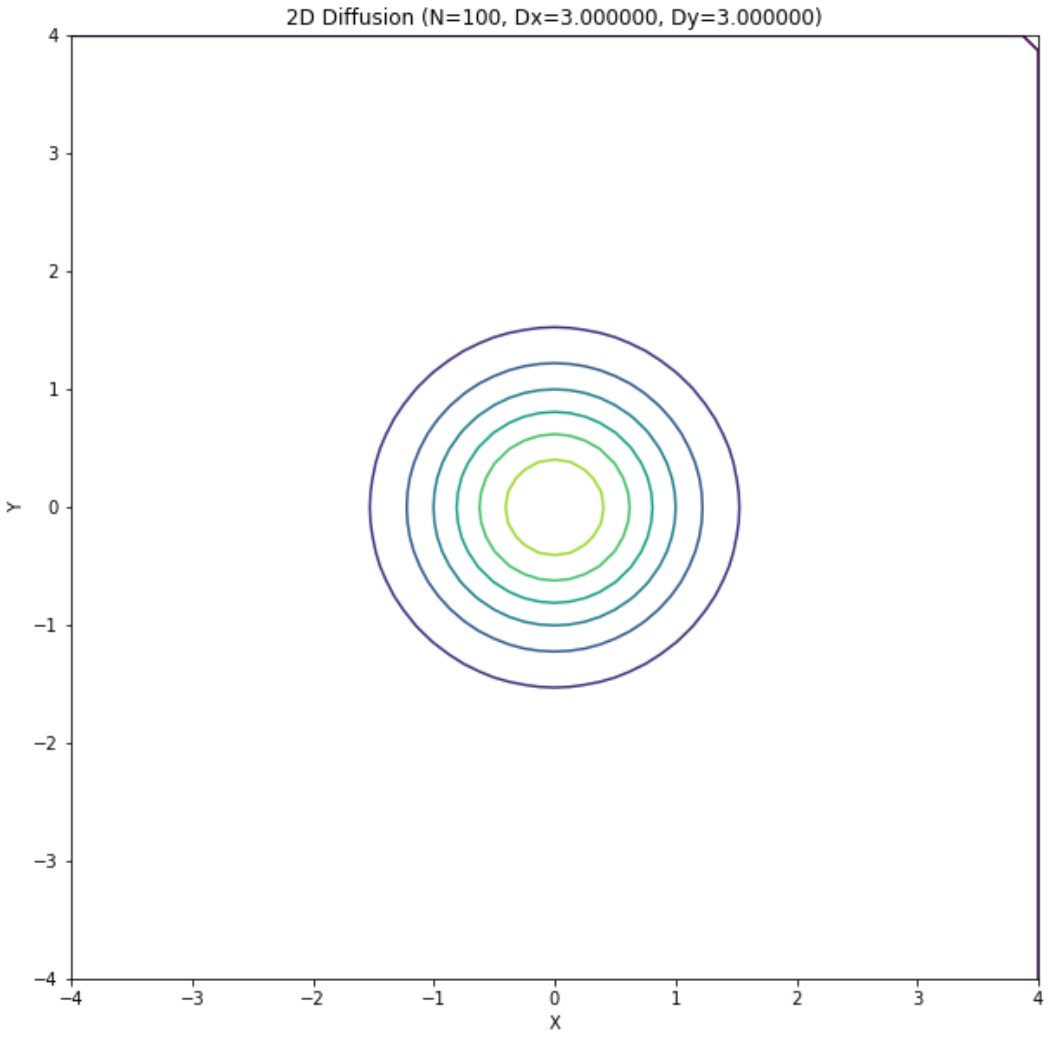


Case 3: Dx = Dy

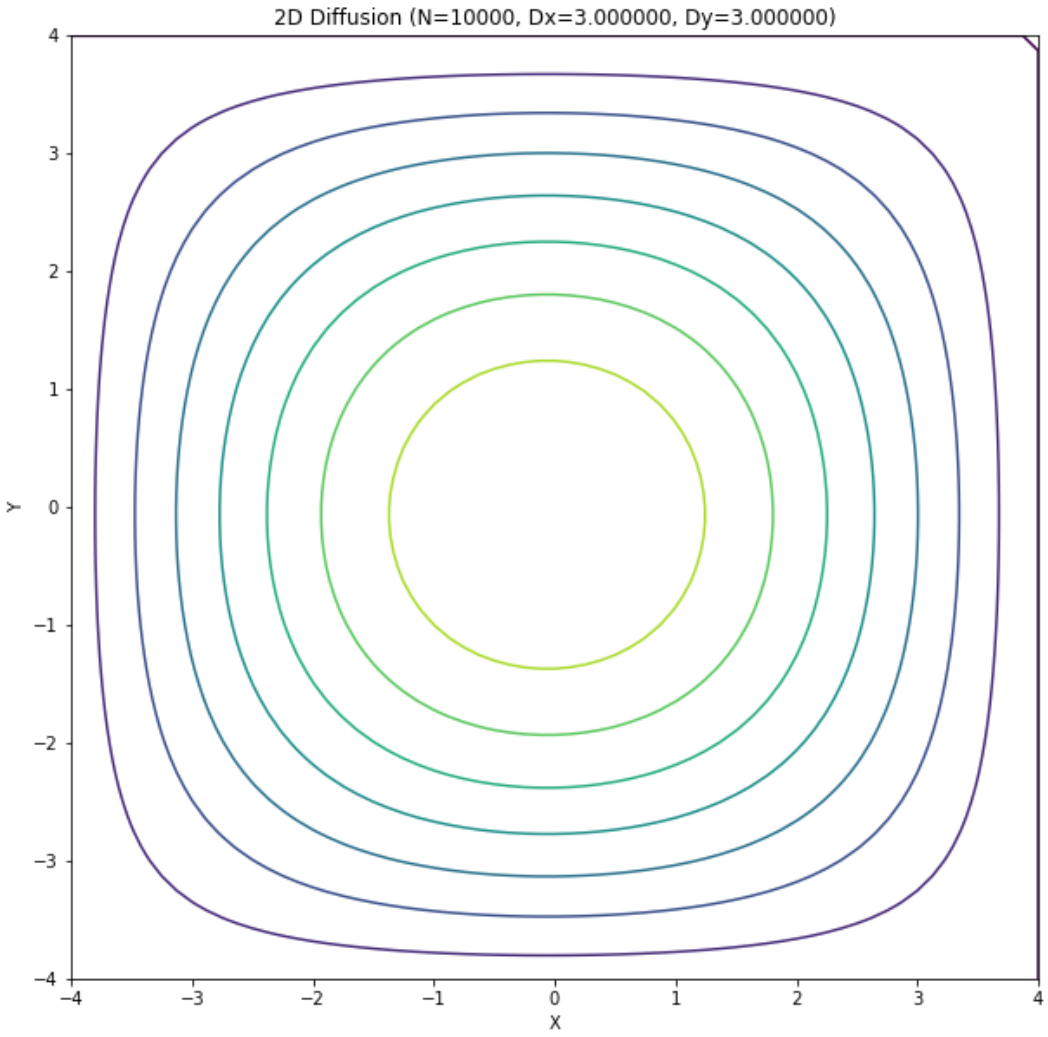
N = 10


2D Diffusion (N=10, Dx=3.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

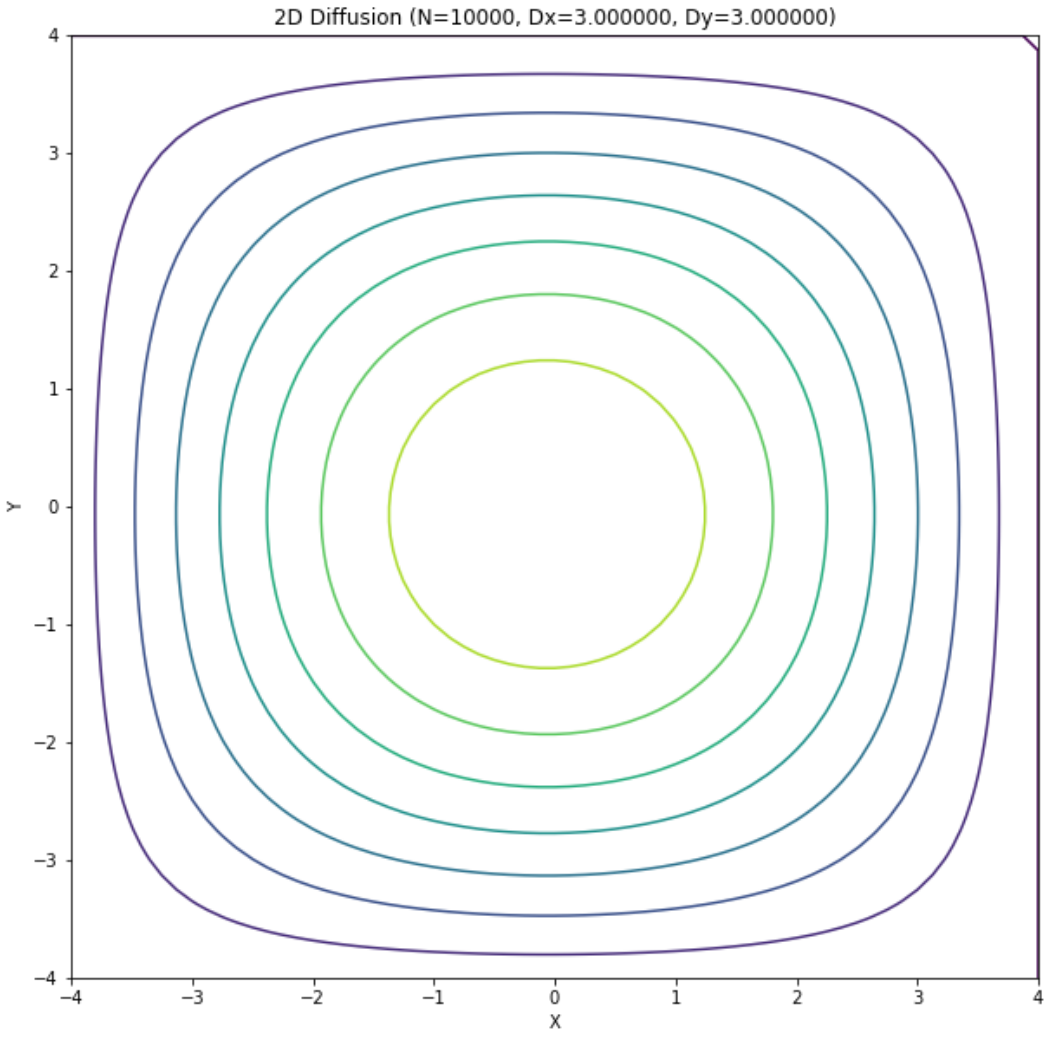
N = 100


2D Diffusion (N=100, Dx=3.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 1000


2D Diffusion (N=10000, Dx=3.000000, Dy=3.000000)
Y
X
4
3
2
1
0
−1
−2
−3
−4
−4
−3
−2
−1
0
1
2
3
4

N = 10000



From the graphs, it is understandable that the molecules spread over larger area as time progresses. The patterns spreads out more in the X direction if Dy is greater and more in the Y direction if Dx is greater.