Computational Physics - PHYS-E0412

Homework Week 1

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In [1]:
```
#importing libraries
import numpy as np
import matplotlib.pyplot as plt
```

(i) Simulating value for D

Function for simulating value for D for a certain amount of walks and steps in the walks

In [2]:
```
def D(walks, steps):
    #Numpy array for storing the x-values of the walk
    x = np.zeros(walks)
    for j in range(0, walks):
        for i in range(1, steps):
            #Drawing step lengths from uniform distribution [-1, 1]
            x[j] += (np.random.rand() - 0.5) * 2

    #Calculating value for D from the x-values
    D = (np.mean(x**2) - np.mean(x)**2) / (steps * 2)
    return D
```

Now if we simulate a value for D with 100 walks with 1000 steps we see that the value for D seems to be about 0.2. However, with these parameter values different runs can give rather different results for D.

In [3]:
```
#steps in walk
steps = 1000

#walks used to calculate D
walks = 100

D(walks, steps)
```

Out[3]: 0.20392292987787303

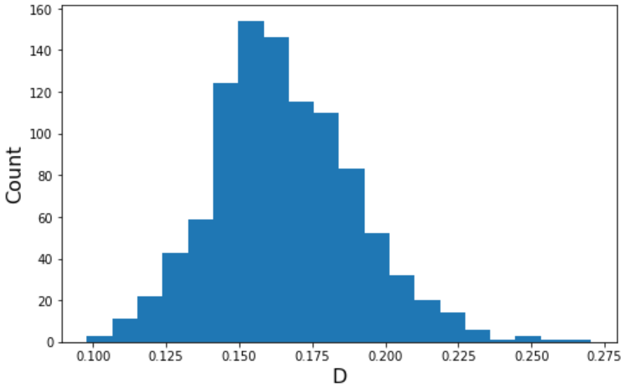
(ii) Distributution of D

Simulating D values and storing them in an array.

In [4]:
```
steps = 1000
walks = 100

#number of D:s calculated
n_D = 1000

#Array for D_values
Ds = np.zeros(n_D)

for i in range(0, n_D):
    Ds[i] = D(walks, steps)
```

Plotting a histogram of D values reveals that the distribution seems to be gaussian.

In [11]:
```
plt.figure(1, (8,5))
plt.hist(Ds, bins = 20)
plt.xlabel("D", size = 16)
plt.ylabel("Count", size = 16)
plt.show()
```



(iii) The mean and the error estimate

In [6]:
```
avg_D = np.mean(Ds)
avg_D
```

Out[6]: `0.16545822709050134`

Mean for the value of D is about 0.165.

The error estimate for a Gaussian distribution can be calculated as

$$\epsilon = \frac{\sigma}{\sqrt{N}}$$

where σ is the standard deviation of D and N the number of diffusion coefficients calculated. This gives us the result of $\epsilon = 0.00078$.

In [7]:
```
std_D = np.std(Ds)
std_D
```

Out[7]: `0.024634832856887414`

In [8]:
```
confidence = std_D / np.sqrt(n_D)
confidence
```

Out[8]: `0.0007790218160531704`

(iiii) Time spent

I used about 4 hours for this exercise. I had to do this twice since it was not at all clear what we should be calculating.