INtroduction to Monte-Carlo methods in Statistical Physics

Monte Carlo methods, or Monte Carlo experiments, are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. The underlying concept is to use randomness to solve problems that might be deterministic in principle.

A Monte Carlo simulation is used to model the probability of different outcomes in a process that cannot easily be predicted due to the intervention of random variables. It is a technique used to understand the impact of risk and uncertainty.

A Monte Carlo simulation is used to tackle a range of problems in many fields including investing, business, physics, and engineering.

Basics:

- What is thermodynamic limit?
- Why need MC?
- Monte-Carlo History
- Gambler's fallacy

For the majority of models of interest today, it has not yet proved possible to find an exact analytic expression for the partition function, or for any other equivalent thermodynamic quantity. In the absence of such exact solutions a number of approximate techniques have been developed including series expansions, field theoretical methods and computational methods.

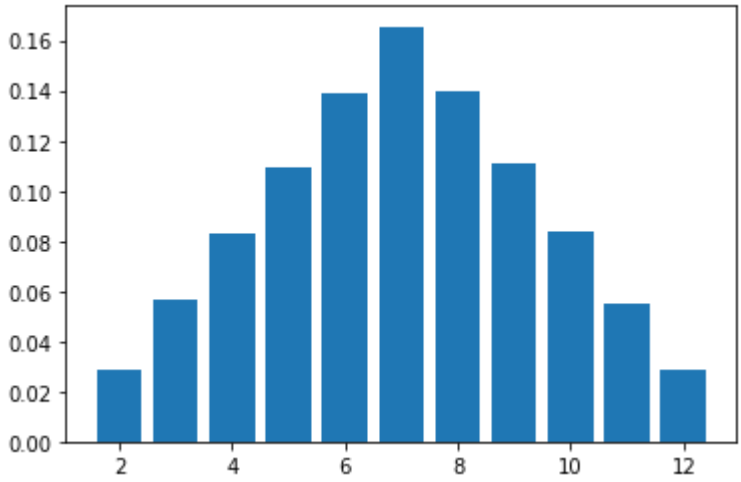
First example of MC method (Roll two dice)

if 2 dices were thrown & there top value were added ,what is the probability of getting a sum of 7 ?

In [38]:
```
import random
import matplotlib.pyplot as plt
import numpy as np

N=100000

outcome=[]

for i in range(N):
    d1=random.randint(1,6)
    d2=random.randint(1,6)
    outcome.append(d1+d2)

valuecount = np.unique(outcome, return_counts=True)

sumall=np.sum(valuecount[1])
```

```
plt.bar(valuecount[0], valuecount[1]/sumall)
```

Out[38]:
```
<BarContainer object of 11 artists>
```



In [34]:
```
np.shape(valuecount)
```

Out[34]:
```
(2, 11)
```

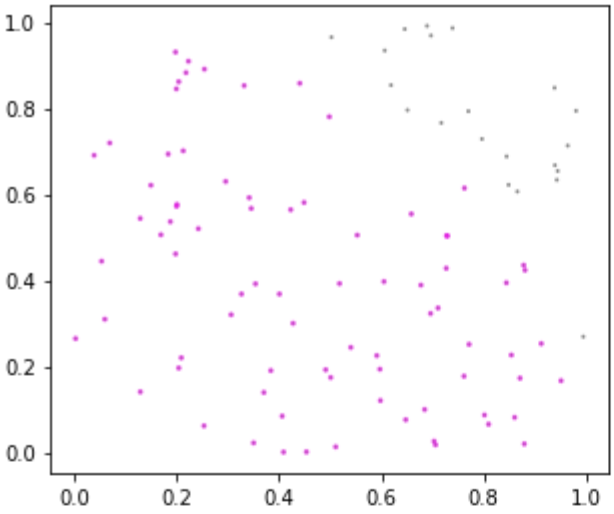
In [88]:
```
## Monte-carlo integration

### Find  pi constant
```

In [94]:
```
import numpy as np

from IPython.display import display, Markdown


N=10000000

pairxy = np.random.rand(N, 2)
accepted = pairxy[pairxy[:,0]**2+pairxy[:,1]**2 < 1]
mcpi = 4*np.shape(accepted)[0]/N


display(Markdown(
   rf"""
$\pi$ is calculated   {mcpi}
"""))
```

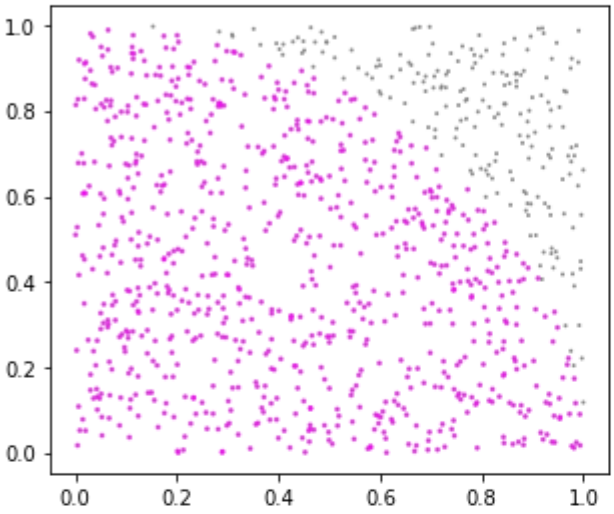
π is calculated 3.1422588

In [1]:
```
import matplotlib.pyplot as plt

import numpy as np

fig, axs = plt.subplots(5,1, figsize=(5,25))


i=0
for N in [100, 1000, 10000, 20000, 100000]:
    pairxy = np.random.rand(N, 2)
```

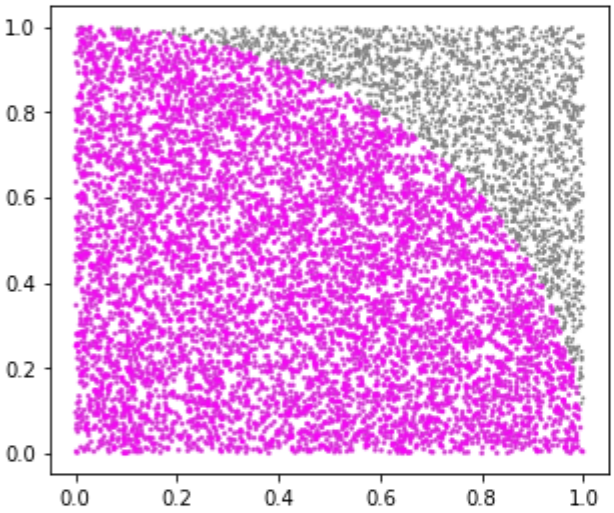
```
    accepted = pairxy[pairxy[:,0]**2+pairxy[:,1]**2 < 1]
    mcpi = 4*np.shape(accepted)[0]/N
    axs[i].scatter(pairxy[:,0], pairxy[:,1], s=4 , alpha=0.9, c='gray', ec='nor
    axs[i].scatter(accepted[:,0], accepted[:,1], s=8, alpha=0.5, c='magenta', e
    message='N is '+str(N)+'\n calculated '+r'$\pi =$'+str(mcpi)
    axs[i].text(x=1.2, y=0.5, s=message, fontsize=16, fontfamily='Serif')
    i=i+1
```



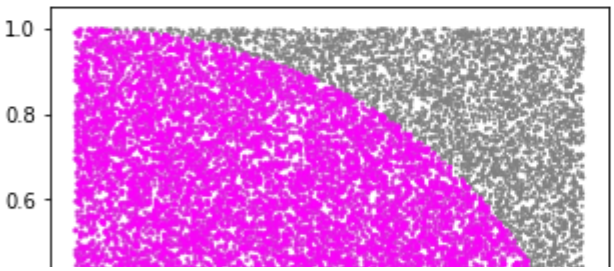
N is 100
calculated $\pi = 3.16$



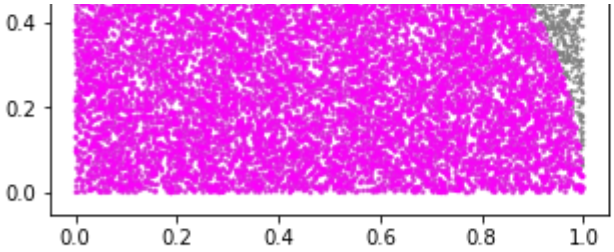
N is 1000
calculated $\pi = 3.188$

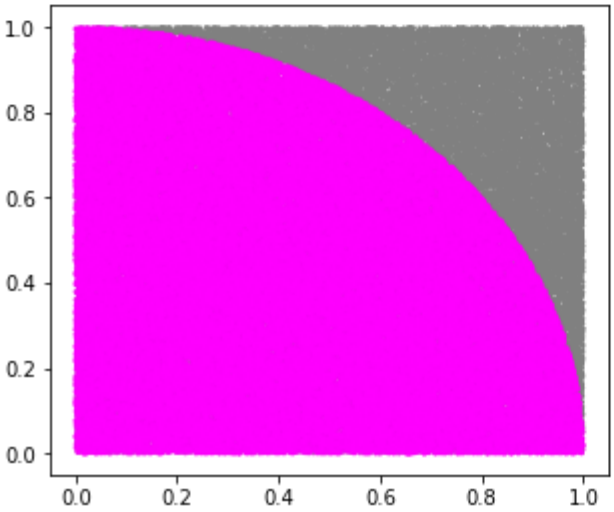


N is 10000
calculated $\pi = 3.1312$



N is 20000
calculated $\pi = 3.1468$





N is 100000
calculated $\pi = 3.14312$

MC Integral

Fist of all review this basics

- Intermediate value theorem
- Mean Value Theorem for Integrals
- central limit theorem

The basic MC strategy

$$I = \int_0^1 f(x)dx$$

$$I \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

from above and central limit theorem one can see $\sigma_I = \sigma_f/\sqrt{(N)}$

above equation reveals two very important aspects of Monte Carlo qudratun;

- First, the uncertainty in the estimate of the integral decrease as $N^{1/2}$
- Second, is that the precision is greater if σ_f is smaller; that is, if f is as smooth as possible.

To gain more insight, consider to limit of f

1) $f(x) = c$ a constant function which average is equal to ... --> MC gives exact estimate 2) for a function with narrow peak and zero value elsewhere --> poor gives poor results

How to imporove ?

Let us imagine multiplying and dividing the integrand by a positive weight function $w(x)$, normalized so that

$\int_0^1 dxw(x) = 1$ and $I = \int_0^1 dxw(x)\frac{f(x)}{w(x)}$ ~~~ use change of variable $y(x) = \int_0^x dx'w(x')$ so that $\frac{dy}{dx} = w(x)$; y(x=0)=0, y(x=1)=1 $

then the integral become

$$I = \int_0^1 dy \frac{f(x(y))}{w(x(y))}$$

The Monte Catlo eduation of this integral proceeds as above, namely ayeraging the values of f/w at a random sampling of points uniformly distributed in y over the interval [0,1]:

$$I \approx \frac{1}{N}\sum_{i=1}^{N}\frac{f(x(y_i))}{w(x(y_i))}$$

The potentiat benefit of the change of &able should now be clw. If we choose a m that behaves approurimately as f does (i-e., it is lage where f is large md small where f is small), then the integrand in above, f /w, can be made very mooth, with a consequent reduction in the variance of the Monte Carlo estimate.

Example

$$\int \frac{1}{1+x^2} = tan^{-1}(x)$$

$\int_0^1 \frac{1}{1+x^2} = tan^{-1}(1) = \pi/4$ & consider $w(x) = 1/3(4-2x)$ to solve integral using simple and wieghted MC

In [28]:
```
import numpy as np

import matplotlib.pyplot as plt

target= np.pi/4
print("exact expected value is  {}\n ======================================".
print(" | number     | error (MC)| error (wieghted)|\n ------------------------

for n in (100, 1000, 5000, 10000, 50000, 100000, 500000, 1000000):
    x=np.random.rand(n)
    f1=1/(1+x**2)
    int1 = np.sum(f1)/n
    y=np.random.rand(n)
    xi = 2-np.sqrt(4-3*y)
    f2=1/(1+xi**2)
    w= (4-2*xi)/3
```

```
    frac = f2/w
    int2=np.sum(frac)/n

    print(" | {:9d}  | {:8.6f}  | {:8.6f} |".format(n, abs(int1-target),  abs(
```

```
exact expected value is  0.7853981633974483
 ========================================
 | number     | error (MC)| error (wieghted)|
 --------------------------------
 |       100  | 0.011533  | 0.001782 |
 |      1000  | 0.001998  | 0.000083 |
 |      5000  | 0.000383  | 0.000268 |
 |     10000  | 0.001566  | 0.000118 |
 |     50000  | 0.000951  | 0.000139 |
 |    100000  | 0.000364  | 0.000127 |
 |    500000  | 0.000259  | 0.000024 |
 |   1000000  | 0.000182  | 0.000036 |
```

Write your main conclusion on above results?

A more general way of understanding why a change of variable is potentially useful is to realize that the nnifonn distribution of points in y implies that the distribution of points in x is $\frac{dy}{dx} = w(x)$. This means that points are concentrated about the **most "importantn"** values of x where w (and hopefully f) is large, and that little computing power is spent on calculating the integrand for "unimportantn values of s where PD and f are small.

MC method for statistical physics

Monte Carlo Methods in Statistical Physics M. E. J. Newman, G. T. Barkema · 1999
https://books.google.com/books?id=HgBREAAAQBAJ&dq=monte+carlo+statistical+physics&hl=en&sa=X&ved=2ahUKEwiahdK27eb

Chapter 1, 2, 3

Outlines:

- Importance Sampling
- Markov processes
- Ergodicity
- Metropolis Algorithm

Compotational Physics (Meredith) Chapter-8

SIMPLE ISING MODEL

$$\mathcal{H} = -J \sum_{<ij>} S_i S_j$$

1D Ising model

$$H = -J \sum_{i=0}^{N-1} S_i S_{i+1} - hS_i$$

At the presence of external field

2D ISING model

 Drawing

We will check that the energy function is working by testing the following obvious conditions:

- The energy for all spin down is –NJ+Nh=N(h–J)
- The energy for all spin up is –NJ–Nh=–N(h+J)
- The energy for alternating spin up and half spin down is (if N is even) +NJ

In [14]:
```
import numpy as np

import matplotlib.pyplot as plt
from sympy.utilities.iterables import multiset_permutations

# number of spins


N=10

config1d=np.random.choice([-1,1], size=(N))
J=1
h=2

test_configuration_3 = +1*np.ones(N)
#this sets even entries to -1
test_configuration_3[::2] = -1


#  PERIODIC 1D SYSTEM
def onedimperiod(config,j, h):
    configShift=np.roll(config,-1)
    # j and h is fixed for all
    totalEnergy=-j*np.sum(config*configShift)-h*np.sum(config)
    magnetization = np.sum(config)/len(config)
    #print("Total enegy is  {}".format(totalEnergy))
    #print("Magnetization is  {}".format(magnetization))

    outputs=[totalEnergy, magnetization]
    return outputs




# NON periodic 1D system
def onedimnonperiod(config,j, h):
    # j and h is fixed for all
```

```
    totalEnergy=-j*np.sum(config[:-1]*config[1:])-h*np.sum(config)
    magnetization = np.sum(config)/len(config)
    #print("Total enegy is  {}".format(totalEnergy))
    #print("Magnetization is  {}".format(magnetization))

    outputs=[totalEnergy, magnetization]
    return outputs

#  How to determine all states?

beta=40
partition=0.0
statesNumber=1
mat=np.empty(N)
for i in range(N):
    startconf=np.ones(N)
    startconf[:i+1]=-1
    for newconf in multiset_permutations(startconf):
        mat=np.vstack((mat,newconf))
        partition += beta*onedimperiod(newconf,1,2)[0]
        statesNumber += 1

print(statesNumber)
```

```
1024
```

Question

What is the energy distribution for the states with similar magnetization

In [15]:

```
import numpy as np
# periodic boundary condition

def energy_ising_1d(configuration,J,h):
    num_spins = len(configuration)
    energy = 0.0
    for i in range(num_spins):
        spini = configuration[i]
        #set the value of spin i+1, make sure to test if i+1<num_spins, and oth
        #you can do this with an if statement if you have to
        ip1 = (i+1)%num_spins
        spinip1 = configuration[ip1]

        energy = energy - J * (spini * spinip1) - h*spini

    return energy

#Check that the energy is correct
test_num_spins = 10
#this should be true for any J, h
test_J = 1
test_h = 2

test_configuration_1 = -1*np.ones(test_num_spins)
test_configuration_2 = +1*np.ones(test_num_spins)

test_configuration_3 = +1*np.ones(test_num_spins)
#this sets even entries to -1
test_configuration_3[::2] = -1
```

```
print("Test Config 1:", test_configuration_1)
print("Energy Config 1:", energy_ising_1d(test_configuration_1,test_J,test_h))
print("Expected Energy Config 1:",test_num_spins*(test_h-test_J))
print()
print("Test Config 2:", test_configuration_2)
print("Energy Config 2:", energy_ising_1d(test_configuration_2,test_J,test_h))
print("Expected Energy Config 2:",-test_num_spins*(test_h+test_J))
print()
print("Test Config 3:", test_configuration_3)
print("Energy Config 3:", energy_ising_1d(test_configuration_3,test_J,test_h))
print("Expected Energy Config 3:",test_num_spins*test_J)
```

```
Test Config 1: [-1. -1. -1. -1. -1. -1. -1. -1. -1. -1.]
Energy Config 1: 10.0
Expected Energy Config 1: 10

Test Config 2: [1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
Energy Config 2: -30.0
Expected Energy Config 2: -30

Test Config 3: [-1.  1. -1.  1. -1.  1. -1.  1. -1.  1.]
Energy Config 3: 10.0
Expected Energy Config 3: 10
```

Metropolis Monte Carlo

1) Calculate energy 2) Choose a random spin index in range [0,N-1], using numpy.random.randint(N) 3) Change that spin from 1 to -1, or -1 to 1 4) Generate a random number r in range 0 to 1, using numpy.random.random() 5) a) if r < min(1,np.exp(-beta*(delta E))): accept move current_energy = energy after flipping You can use the python command `pass` to represent not doing anything b) otherwise, reject move change that spin back to it's old value don't update the current energy

In [16]:
```
#set a seed for the random number generator here. For a given seed, all of you
random_seed = 1
np.random.seed(random_seed)

def metropolis_mc_slow(n_steps, n_lattice_sites, beta, J, h, debug=False,save_
    # we can start with a random configuration of size n_lattice_sites by gene
    #    of zeros and twos, then subtracting 1, the following does that, do yo
    #   with this function in an empty box if you don't
    configuration = 2*np.random.randint(2, size=n_lattice_sites) - 1
    average_spins = []

    if debug is True:
        print("Starting configuration:",configuration)

    current_energy = energy_ising_1d(configuration,J,h)
    for i in range(n_steps):

        spin_to_change = np.random.randint(n_lattice_sites)
        # Change configuration[spin_to_change] to it's opposite value (1->-1,
        # There is a very simple mathematical operation that does this, regarl
        configuration[spin_to_change] *= -1

        energy_flip = energy_ising_1d(configuration,J,h)
```

```
        r = np.random.random()
        #do metropolis test w/ this random nubmer r
        if r<min(1,np.exp(-beta*(energy_flip-current_energy))):
            current_energy = energy_flip
        else:
            #set spin back the same way you did before
            configuration[spin_to_change] *= -1

        #this computes the average of the spin observable
        average_spin = configuration.mean()

        if i%save_freq == 0:
            average_spins.append(average_spin)

        if debug and i%10==0:
            print("%i: "%i,configuration,"Energy:",current_energy,"Spin:",avera

    return average_spins

#do a test high temperature simulation
print("High temperature:")
average_spins = metropolis_mc_slow(n_steps=100, n_lattice_sites=10, beta=0.1, .
#do a test on a low temperature simulation
print("Low temperature:")
average_spins = metropolis_mc_slow(n_steps=100, n_lattice_sites=10, beta=1, J=1
```

```
High temperature:
Starting configuration: [ 1  1 -1 -1  1  1  1  1  1 -1]
0:  [-1  1 -1 -1  1  1  1  1  1 -1] Energy: -6.0 Spin: 0.2
10:  [-1  1  1 -1 -1  1  1  1  1  1] Energy: -10.0 Spin: 0.4
20:  [ 1 -1  1  1  1 -1  1 -1  1  1] Energy: -6.0 Spin: 0.4
30:  [ 1 -1 -1  1  1  1 -1 -1  1  1] Energy: -6.0 Spin: 0.2
40:  [-1 -1 -1 -1  1  1  1 -1 -1  1] Energy: 2.0 Spin: -0.2
50:  [-1  1 -1  1 -1  1 -1 -1 -1 -1] Energy: 10.0 Spin: -0.4
60:  [-1  1  1  1  1  1  1  1  1 -1] Energy: -18.0 Spin: 0.6
70:  [-1 -1 -1 -1 -1 -1  1 -1  1 -1] Energy: 10.0 Spin: -0.6
80:  [ 1  1  1  1 -1 -1  1  1 -1 -1] Energy: -6.0 Spin: 0.2
90:  [-1  1  1 -1  1 -1 -1  1  1 -1] Energy: 2.0 Spin: 0.0
Low temperature:
Starting configuration: [-1 -1  1 -1 -1 -1  1 -1  1  1]
0:  [ 1 -1  1 -1 -1 -1  1 -1  1  1] Energy: 2.0 Spin: 0.0
10:  [ 1 -1  1  1  1  1  1  1  1  1] Energy: -22.0 Spin: 0.8
20:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
30:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
40:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
50:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
60:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
70:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
80:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
90:  [1 1 1 1 1 1 1 1 1 1] Energy: -30.0 Spin: 1.0
```

In [119…

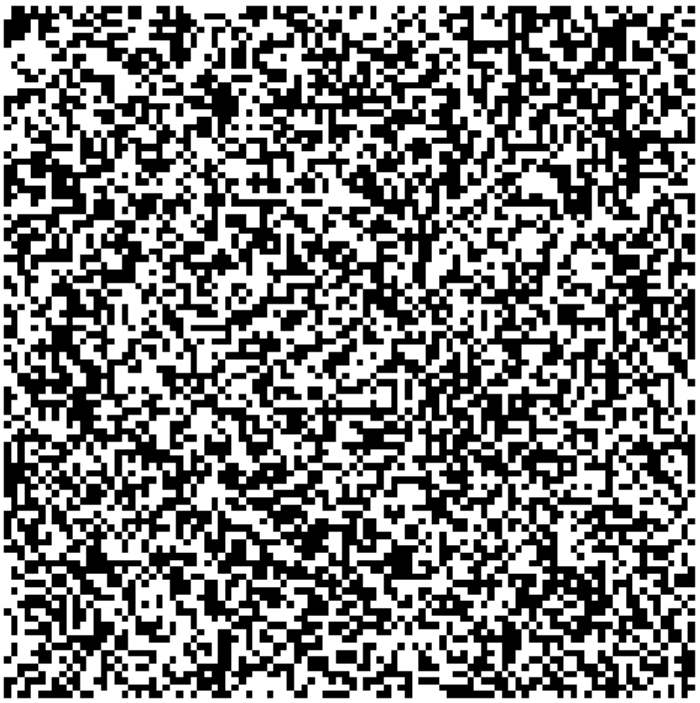
```
%matplotlib notebook

import numpy as np
import matplotlib.pyplot as plt
from matplotlib import animation


N=100  #The discretization parameter. There are N^2 points.
```

```
T = 0.001   #The temperature of the system.


#setting up the figure
fig = plt.figure()
plt.axis('off')
initial_spins = np.random.choice([-1,1], size=(N,N))
initial_spins[0,0] = -1
im = plt.imshow(initial_spins, cmap = 'gray')
```

In [121…

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import animation


N=100  #The discretization parameter. There are N^2 points.
T = 0.001   #The temperature of the system.


#setting up the figure
fig = plt.figure()
plt.axis('off')
initial_spins = np.random.choice([-1,1], size=(N,N))
initial_spins[0,0] = -1
im = plt.imshow(initial_spins, cmap = 'gray')


def animate(i):
    for _ in range(0, 100):
        initial_spins = np.random.choice([-1,1], size=(N,N))
```

```
        im = plt.imshow(initial_spins, cmap = 'gray')

    return [im]



anim = animation.FuncAnimation(fig, animate,blit=True)
```



In [116…

```
%matplotlib notebook

import numpy as np
import matplotlib.pyplot as plt
from matplotlib import animation


N=100  #The discretization parameter. There are N^2 points.
T = 0.001   #The temperature of the system.

flips_per_frame = N*N//20
number_of_frames = 100000

#setting up the figure
fig = plt.figure()
plt.axis('off')
initial_spins = np.random.choice([-1,1], size=(N,N))
initial_spins[0,0] = -1
im = plt.imshow(initial_spins, cmap = 'gray')

# animation function.  This is called sequentially
```

```
def animate(i):
    for _ in range(0, flips_per_frame):
         i = np.random.randint(0,N)
         j = np.random.randint(0,N)

         spins = im.get_array()
         # %N gives periodic boundary conditions.
         deltaE = 2*spins[i,j]*(spins[(i+1)%N,j] + spins[i,(j+1)%N]
                                + spins[(i-1)%N,j] + spins[i,(j-1)%N])

         if deltaE < 0:
             spins[i,j] *= -1

         elif  np.random.uniform() < np.exp(-deltaE/T):
             spins[i,j] *= -1

    return [im]

anim = animation.FuncAnimation(fig, animate,
                               frames=number_of_frames, interval=20, blit=True
```

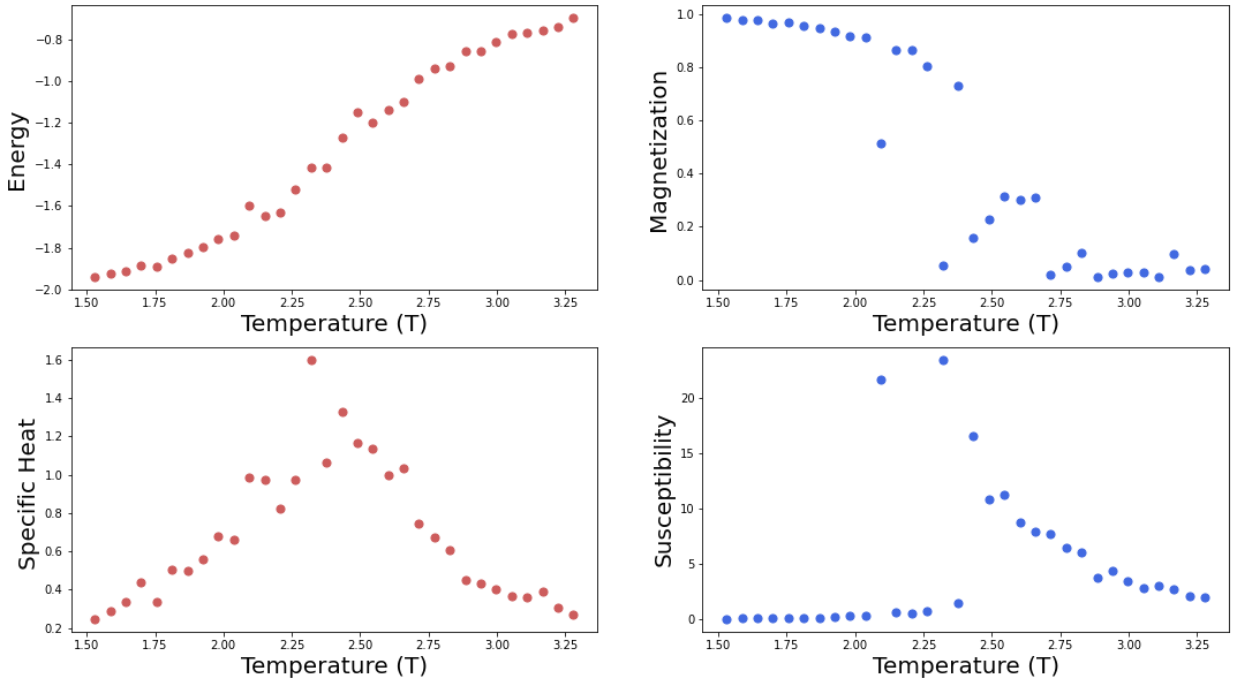
In [111…

```
import numpy as np
from numpy.random import rand
import matplotlib.pyplot as plt
from scipy.sparse import spdiags,linalg,eye


##  BLOCK OF FUNCTIONS USED IN THE MAIN CODE
#-----------------------------------------------------------------------
```

```
def initialstate(N):
    '''
    Generates a random spin configuration for initial condition
    '''
    state = 2*np.random.randint(2, size=(N,N))-1
    return state



def mcmove(config, beta):
    '''
    Monte Carlo move using Metropolis algorithm
    '''

    for i in range(N):
        for j in range(N):
                a = np.random.randint(0, N)
                b = np.random.randint(0, N)
                s =  config[a, b]
                nb = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b]
                cost = 2*s*nb

                if cost < 0:
                    s *= -1
                elif rand() < np.exp(-cost*beta):
                    s *= -1
                config[a, b] = s
    return config



def calcEnergy(config):
    '''
    Energy of a given configuration
    '''
    energy = 0

    for i in range(len(config)):
        for j in range(len(config)):
            S = config[i,j]
            nb = config[(i+1)%N, j] + config[i,(j+1)%N] + config[(i-1)%N, j] +
            energy += -nb*S
    return energy/2.  # to compensate for over-counting



def calcMag(config):
    '''
    Magnetization of a given configuration
    '''
    mag = np.sum(config)
    return mag




## NOTE: change these parameters for a smaller and faster simulation
#---------------------------------------------------------------------
```

```
nt      = 32         #  number of temperature points
N       = 10         #  size of the lattice, N x N
eqSteps = 2**8       #  number of MC sweeps for equilibration
mcSteps = 2**9       #  number of MC sweeps for calculation


T       = np.linspace(1.53, 3.28, nt);
E,M,C,X = np.zeros(nt), np.zeros(nt), np.zeros(nt), np.zeros(nt)
n1, n2  = 1.0/(mcSteps*N*N), 1.0/(mcSteps*mcSteps*N*N)
# divide by number of samples, and by system size to get intensive values









#  MAIN PART OF THE CODE
#----------------------------------------------------------------------


for tt in range(nt):
    config = initialstate(N)         # initialise

    E1 = M1 = E2 = M2 = 0
    iT=1.0/T[tt]; iT2=iT*iT;

    for i in range(eqSteps):         # equilibrate
        mcmove(config, iT)           # Monte Carlo moves

    for i in range(mcSteps):
        mcmove(config, iT)
        Ene = calcEnergy(config)     # calculate the energy
        Mag = calcMag(config)        # calculate the magnetisation

        E1 = E1 + Ene
        M1 = M1 + Mag
        M2 = M2 + Mag*Mag
        E2 = E2 + Ene*Ene


    # divide by number of sites and iteractions to obtain intensive values
    E[tt] = n1*E1
    M[tt] = n1*M1
    C[tt] = (n1*E2 - n2*E1*E1)*iT2
    X[tt] = (n1*M2 - n2*M1*M1)*iT









#  plot the calculated values
#----------------------------------------------------------------------
```

```
f = plt.figure(figsize=(18, 10)); #


sp =  f.add_subplot(2, 2, 1 );
plt.scatter(T, E, s=50, marker='o', color='IndianRed')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Energy ", fontsize=20);          plt.axis('tight');


sp =  f.add_subplot(2, 2, 2 );
plt.scatter(T, abs(M), s=50, marker='o', color='RoyalBlue')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Magnetization ", fontsize=20);   plt.axis('tight');


sp =  f.add_subplot(2, 2, 3 );
plt.scatter(T, C, s=50, marker='o', color='IndianRed')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Specific Heat ", fontsize=20);   plt.axis('tight');


sp =  f.add_subplot(2, 2, 4 );
plt.scatter(T, X, s=50, marker='o', color='RoyalBlue')
plt.xlabel("Temperature (T)", fontsize=20);
plt.ylabel("Susceptibility", fontsize=20);   plt.axis('tight');
```



In [ ]: