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1  # -*- coding: utf-8 -*-
2  """
3  Created on Sun Jan  5 11:47:14 2020
4
5  @author: Alexm
6  """
7
8  import matplotlib
9  #matplotlib.use("Qt4Agg") #take this out on jupyter
10 import numpy as np
11 import matplotlib.pyplot as plt
12 import matplotlib.animation as animation
13 from numpy.random import rand
14 %matplotlib notebook
15 print('Alexandra Mulholland 17336557')
16 print('Part 4: Animation of the configurations')
17
18 #Part 4- Simulation of the configuration of the matrix
19 #We will be using a slightly different Metropolis algorithm for the sake of simplicity
20 #For a ferromagnetic material at constant temperature and no external magnetic field influence
21
22
23 #Here, as before, we will randomly select a point, s, in the lattice and identify the 4 neighbours to said point.
24
25 #The spin product is again calculated- although this time outside of the definition for the energy change (EC), unlike in the
26 #codes for parts 1,2 and 3.
27
28 #ec is the spin product (spinproduct) and exchange energy (J) product, which is later used to find the energy change EC upon a lattice point's spin
29 #being flipped.
30
31 #ec is used in the Metropolis algorithm, which has been altered from parts 1,2 and 3.
32
33 #Initial configuration is produced: an N x N lattice of spins being either 1 or -1
34
35 def randomstate(N):
36     state = 2*np.random.randint(2, size=(N,N))-1
37     return state
38
39 def Ising(a,b):
40     s = config[a,b]
41     naybor = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b] + config[a,(b-1)%N]
42     spinproduct = s * naybor
43     ec = -J*spinproduct
44     return ec
45 #The Metropolis algorithm (altered). Rather than elaborating on this within the report, I will simply
46 #explain the differences in said algorithm here.
47     #A random point within the lattice is selected
48     #The spin of said point is determined and flipped regardless of energy change magnitude
49     #The energy change before and after the flip is calculated (finish-start)
50     #As with the previous codes, a random number between 0 and 1 is generated
51     #If this number is greater than the Boltzmann factor, the spin is then flipped again
52     #This contrasts again to previous codes where if this number was LESS than the Boltzmann factor, the spin was flipped
53     #This change still makes logical sense: This is due to the fact that the spin had been
54     #flipped regardless of what was energetically favourable
55
56 #The single asterisk form (*args) is used to pass a non-keyworded, variable-length argument list"
57 #Without this, the animation would not change. It calls the parameters listed underneath
58 def moncar(*args):
59     a = np.random.randint(0,N) #random lattice point is chosen, coordinate (a,b)
60     b = np.random.randint(0,N)
61     start = Ising(a,b) #its spin product with its neighbours is found and multiplied by the exchange energy
62     config[a,b] *= -1 #flipping the spin of chosen point
63     finish = Ising(a,b) #Final spin of chosen point x -J x spin of neighbours
64     EC = finish-start #energy change as a result of the flipped spin
65     if(rand() > np.exp(-EC/T)): #If this energy change results in the random number generated being greater than the boltzmann constant,
66         config[a,b] *= -1 #the spin is flipped again (back to its original spin). Otherwise, it remains in its flipped spin state
67     mesh.set_array(config.ravel()) #returns the array, flattened. "1D array with all the input-array elements and

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with the same type as it"
68     return config
69
70
71
72 T = 1.0 #Temperature-- again, 1/T=beta
73 N = 20 #NxN matrix
74 J = 1 #Exchange energy
75 stepsmoncar = 2000 #Number of times the Metropolis algorithm will be executed
76 config = randomstate(N) #Initial, random matrix of spins
77
78 #Performing the simulation
79 fig = plt.figure(figsize=(10, 10), dpi=70) #figure size and dpi is how many pixels the figure comprises
80 fig.suptitle("Animation of the execution of the Metropolis algorithm for a 20x20 lattice", fontsize=15)
81 plt.title("For T = %0.1fK" %T, fontsize=10)
82 plt.gca().axes.get_yaxis().set_visible(False)
83 plt.gca().axes.get_xaxis().set_visible(False)
84 X, Y = np.meshgrid(range(N), range(N)) #grid size
85 mesh = plt.pcolormesh(X, Y, config, cmap = plt.cm.winter, vmin=-1, vmax=1) #vmin and vmax define the data range
86 k = animation.FuncAnimation(fig, moncar, frames = stepsmoncar, interval = 5, blit = True)
87 plt.show()

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