

SETUP

```

1 #!/bin/env python
2 #
3 # 11/03/19
4 # Chris Self
5 #
6 import sys,time,json
7 import numpy as np
8 from mpi4py import MPI
9 # import ptmpi packages
10 import ptmpi
11 from ptmpi import swaphandler as PtMPI
12 from ptmpi import filehandler as PtMPI_out
13
14 if __name__ == '__main__':
15
16     # =====
17     # setup
18     # =====

```

defining the parameters of the system to be modelled

```

21 # system parameters:
22 # standard 2d Ising model on a square lattice
23 # Hamiltonian:  $H = -J \sum_i \sum_j \langle i,j \rangle \sigma_i \sigma_j - K \sum_i \sigma_i$ 
24  $L = 10$ 
25  $J = 1$  # spin-spin coupling
26  $K = 0.1$  # external magnetic field coupling

```

```

27 # output file name
28 output_name = '2d-ising'

```

```

31 # fix total number of pt swap rounds
32 number_swaps = 1000
33
34 # each process has a copy of the same temperature set
35 T_logset = np.linspace(-1,2,20)
36 betas = np.array([ 1.*10**(-bb) for bb in T_logset ])

```

defining the parameters of the parallel tempering

```

37 # =====
38 # initialisation
39 # =====

```

```

41 # initialise the MPI environment
42 comm = MPI.COMM_WORLD
43 rank = comm.Get_rank()
44 if not len(betas)==comm.Get_size():
45     print('Error, the number of temperatures is different than the number of chains.\n\
46         +\'Aborting simulation.\')

```

initialise the MPI environment and this process's copy of the ptmpi object

```

47 # announce start
48 if rank==(comm.Get_size()-1):
49     print(sys.argv[0]+' initialising...\n'+ '-'*40)
50 comm.Barrier()
51 begin_time = time.time()

```

```

54 # initialise ptmpi controller object
55 mpi_pt_handler = PtMPI.swaphandler( comm,rank,number_swaps=number_swaps,verbose=True )

```

```

58 # initialise this process's copy of the system
59 print(str(rank)+' : initialising copy of the system')
60 ising_spins = 2*np.random.randint(2,size=(L,L))-1 # begin in a random state
61 # compute starting energy
62 E = 0
63 for site_i in range(L):
64     for site_j in range(L):
65         E += -K*ising_spins[site_i,site_j]
66         E += -J*ising_spins[site_i,site_j]*ising_spins[(site_i+1)%L,site_j]
67         E += -J*ising_spins[site_i,site_j]*ising_spins[site_i,(site_j+1)%L]

```

initialising the copy of the system this process holds

```

68 # =====
69 # mcmc and pt loop
70 # =====

```

```

72 # open output file array
73 if rank==(comm.Get_size()-1):
74     print('initialising shared output files...')
75     with PtMPI_out.filehandler(comm,filename='output/timeseries'+output_name) as out_file:
76         # wrap an array in output file
77         with out_file.wrap_array():

```

ptmpi context managers handle the shared output files

```

78         # store start time
79         start_time = time.time()
80         start_block_time = time.time()

```

```

82 # parallel tempering swaps are the unit of our monte-carlo time and each unit
83 # of time corresponds to a Metropolis sweep i.e.  $O(L^2)$  metropolis steps
84 for swaps_counter in range(number_swaps):

```

```

85     # print progress update every X bins
86     progress_time_unit = max(10,int(np.floor(number_swaps/100.)))
87     make_noise = ((rank==(comm.Get_size()-1)) and (swaps_counter%progress_time_unit==0))
88     if make_noise:
89         end_block_time = time.time()
90         print('-'*15)
91         print('process 0 at swaps_counter '+str(swaps_counter))
92         print('last block of '+str(progress_time_unit)+' bins took: '\
93             + '{0:.3g}'.format(end_block_time-start_block_time)+' seconds')
94         start_block_time = time.time()

```

MAIN LOOP

current temperature of this process is queried from ptmpi object

index of output file (temperature index) is passed to ptmpi file handler when outputting data

data needed to decide whether to swap or not is passed to ptmpi

```

100 # mcmc sweep
101 #
102 for mc_step in range(L**2):
103     site_i,site_j = np.random.randint(L,np.random.randint(L))
104
105     # compute change in energy
106     delta_E = 2.*J*ising_spins[site_i,site_j]
107     delta_E += 2.*J*ising_spins[site_i,site_j]*ising_spins[(site_i+1)%L,site_j]
108     delta_E += 2.*J*ising_spins[site_i,site_j]*ising_spins[site_i,(site_j+1)%L]
109     delta_E += 2.*J*ising_spins[site_i,site_j]*ising_spins[site_i,(site_j-1)%L]
110
111     # accept or reject
112     beta_index = mpi_pt_handler.get_current_temp_index()
113     acceptance_probability = min(1,np.exp(-betas[beta_index]*delta_E))
114     if np.random.random()<acceptance_probability:
115         ising_spins[site_i,site_j] = -1*ising_spins[site_i,site_j]
116         E += delta_E

```

a sweep of MCMC updates in the system

```

117 # output current state
118 beta_index = mpi_pt_handler.get_current_temp_index()
119 output_data = {"beta":betas[beta_index],"energy":E,"magnetisation":np.sum(ising_spins)}
120 out_file.dump(beta_index,output_data)

```

output data to the relevant file

```

121 # parallel tempering swap step
122 #
123 try:
124     curr_beta_index = mpi_pt_handler.get_current_temp_index()
125     alt_beta_index = mpi_pt_handler.get_alternative_temp_index()
126     success_flag = mpi_pt_handler.pt_step(E,betas[curr_beta_index],betas[alt_beta_index])
127 except PtMPI.NoMoreSwaps:
128     print('No more swaps attempted at the end of pt_subsets')
129     break

```

ptmpi object communicates with neighbor processes to decide

whether to swap or not

```

131 # record the run time of the stage and add the runtime to the task_spec
132 run_time = (time.time()-begin_time)
133 if rank==(comm.Get_size()-1):
134     print('total runtime: '+str(run_time)+' seconds.')

```