Project 1

Path to the source code: `/home/d/dx/dxj4360/Project1`

Introduction

Statistical Background

- `Ferromagnetic` materials will tend to have ordered magnetic dipole momentum when exposed to external magnetic field and keep `ordered phase` afterwards.
- `Paramagnetic` materials can be weakly induced by external magnetic field but will revert to `disordered phase` when the external field is removed.
- `Phase transition` is when the microstates of materials change between ordered phase and disordered phase.
- A `microstate` is a specific microscopic configuration of a thermodynamic system.
- Due to thermal fluctuations, each mircostate has a certain `probability` of occurrence, which is the possibility of the microscopic configuration: $P(x) = \frac{1}{Z}e^{-\beta H(x)}$. The total probability of all configurations is 1.
- `Statistical average`, in my understanding, is the ensemble of all possible states, which equals the mean value of all microstates of a system.

Ising Model

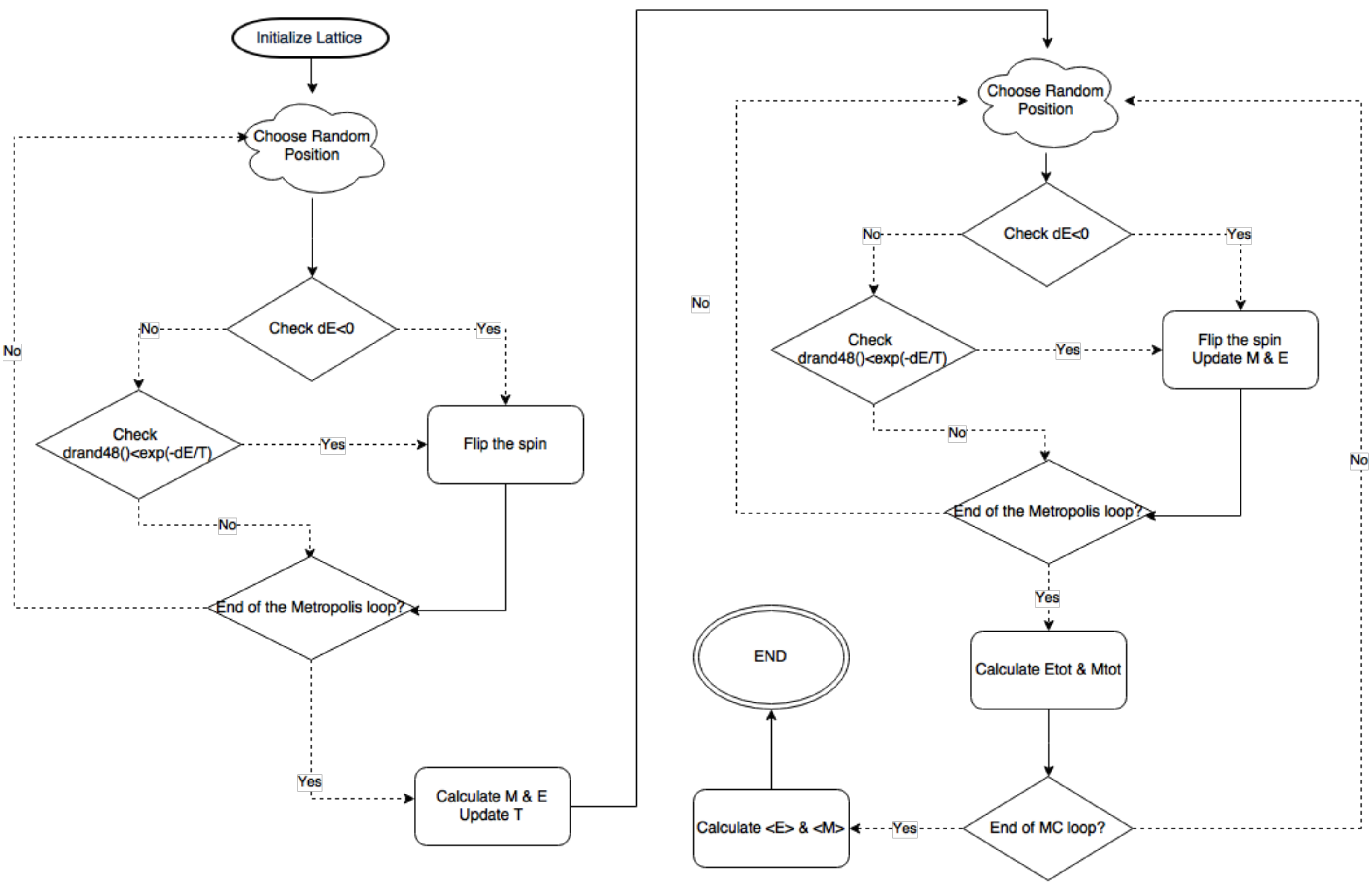
- The `Ising Model` is a mathematical model in statistical mechanics. It uses discrete variables to represent magnetic dipole moments of atomic `spins`, whose `possible value` is ± 1.
- The `energy` of a configuration σ is given by the Hamiltonian function: $H(\sigma) = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - h\sum_j \sigma_j$.
- For a system of N spins $(N = L \times L)$, there are 2^N microstates.

Monte Carlo method

- For a 2-dimensional square lattice at the no external magnetic field case $(H = 0)$, we have
    - $L = 20$: the total number of sites on the lattice,
    - $\sigma_j \in \{-1, +1\}$: an individual spin site on the lattice, $j = 1, \ldots, L$,
    - $S \in \{-1, +1\}^L$: state of the system.

- Since there is no external field, the Hamiltonian function is thus, $H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$.
- The probability function has an actual statistical weight. In a discrete case that the phase space a computer algorithm will generate is finite, we need to use `importance sampling` for better estimating the properties of a particular distribution.
- The total energy E_{flip} can be calculated from the Hamiltonian given earlier: $\langle E \rangle = \frac{1}{2} \langle -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \rangle$

Pseudocode



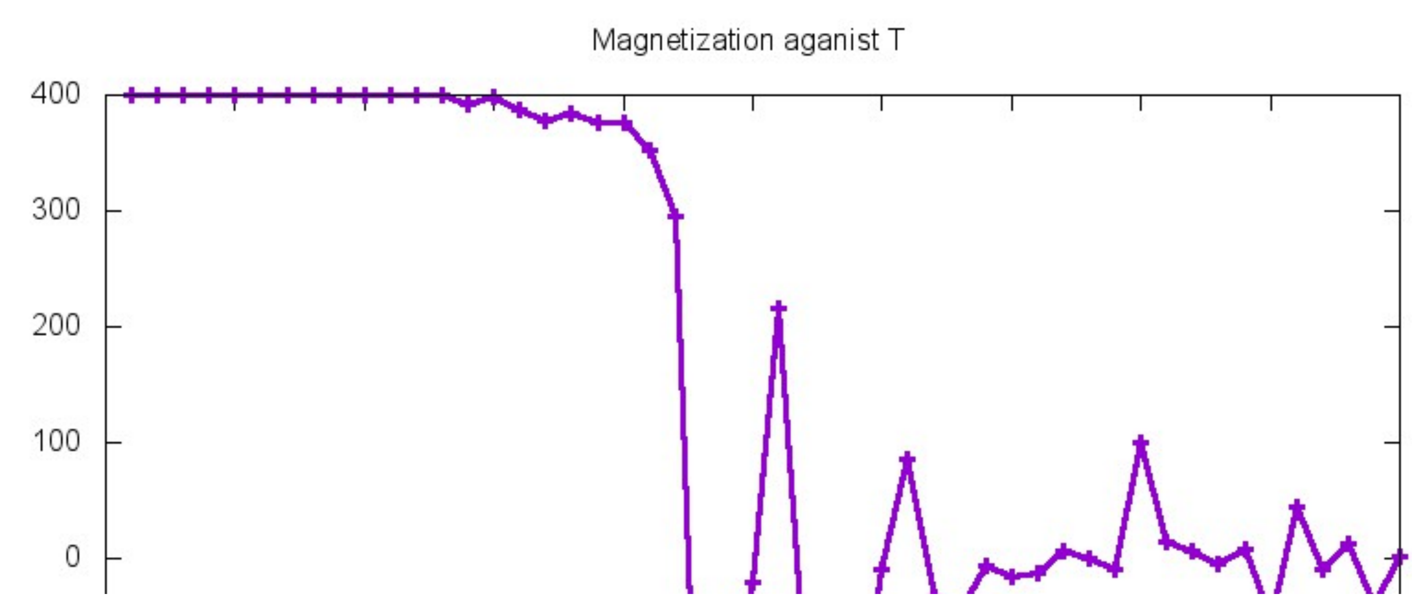
Fortran code

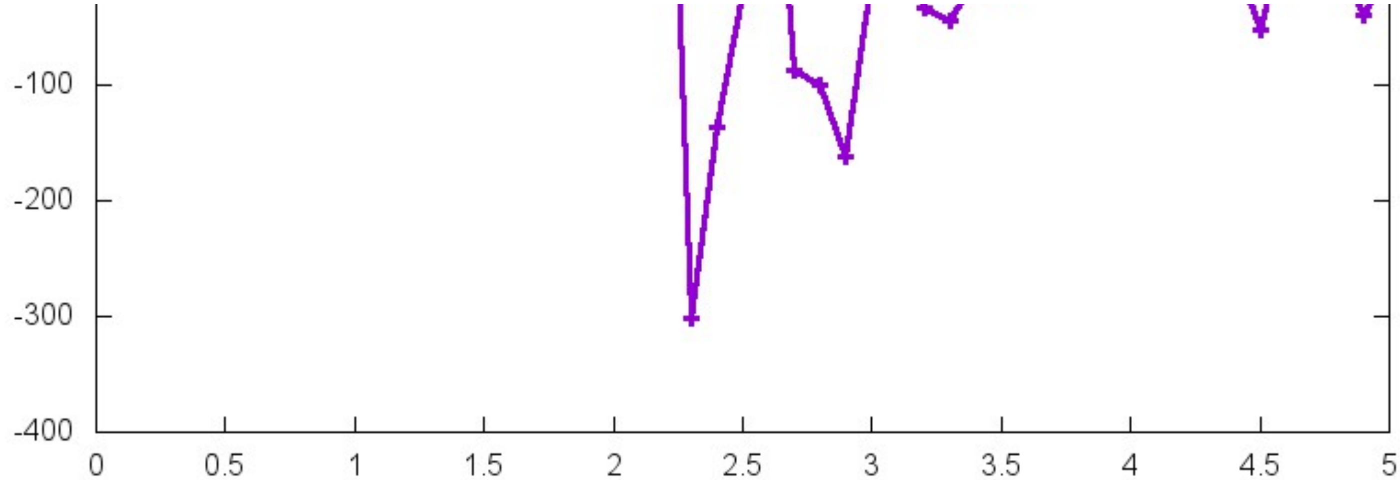
```
program ising_model_2d
    implicit none
    real*8, external :: drand48
    integer :: i,j,x,y,nmc=10000,n,transient
    real*8 :: T,e,M,dE, Etot=0,Mtot=0, E_avg=0,M_avg=0,norm,temp_e
```

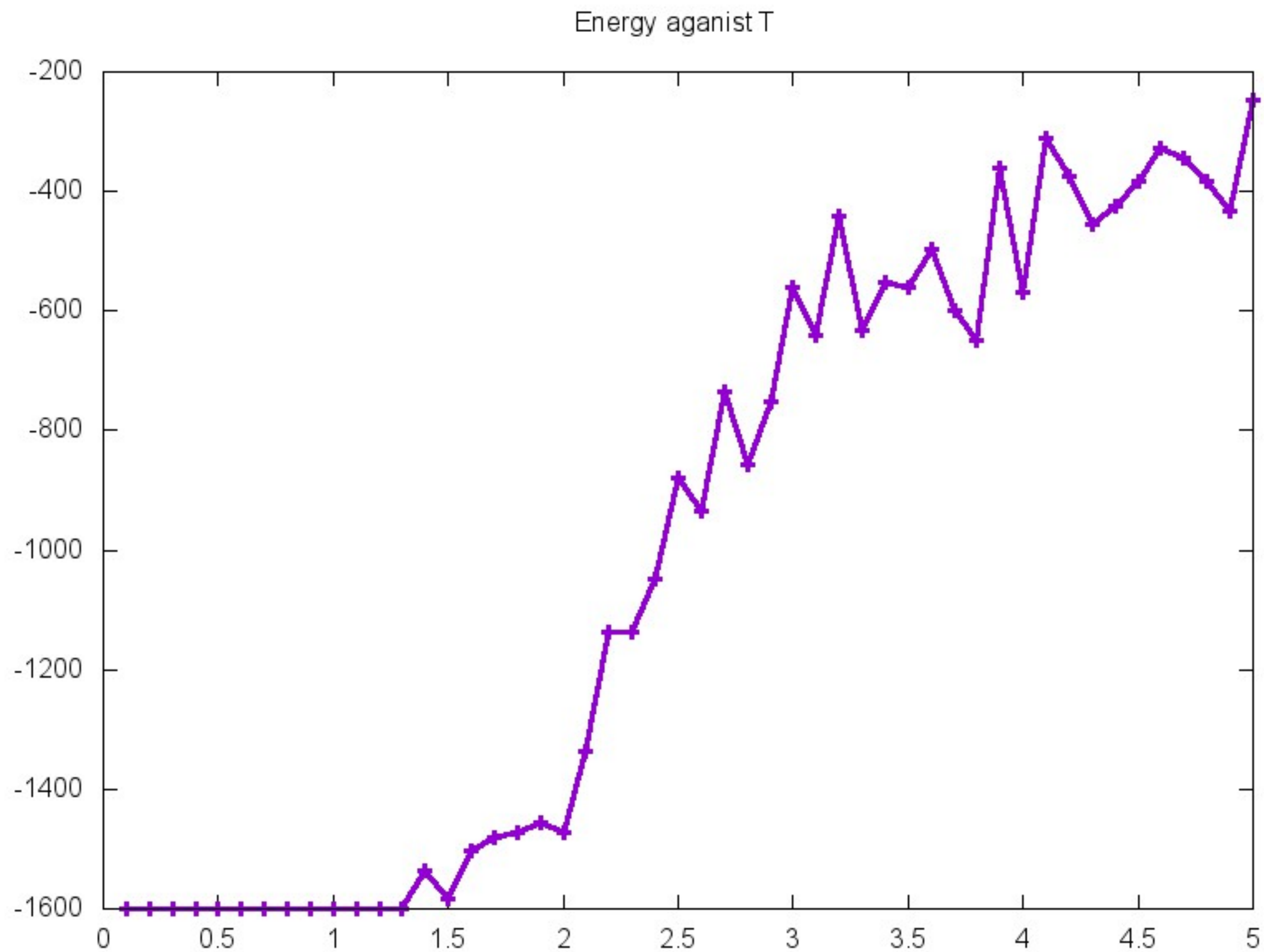
```fortran
    integer, dimension(2) :: lat(20,20)

    norm =1.d0/4.0D6
    ! initialize the lattice
    ! python: lat.append(random.choice([1,-1],size=L*L))
    do x=1,20
        do y=1,20
            if (drand48().ge.0.5) then
                lat(x,y)=1
            else
                lat(x,y)=-1
            end if
        enddo
    enddo

    do T=5.0,0.0,-0.1
        do transient=1,1000
            do n=1,400
                ! choose random pos
                x=floor(drand48()*20)+1
                y=floor(drand48()*20)+1
                ! check energy
                ! merge function is fortran version of lambda function. merge(resA,resB,c
                e=-1*lat(x,y)*(lat(merge(20,x-1,x<2),y)+lat(merge(1,x+1,x>19),y)+lat(x,me
                dE=-2*e
                if (dE.lt.0 .or. drand48().le.exp(-dE/T)) then
                    ! flip
                    lat(x,y)=-lat(x,y)
                end if
            enddo
        enddo
        ! ceil energy calculation in python:
        !   E=-1*sum(multiply(lat,roll(lat,1,axis=0)+roll(lat,-1,axis=0)+roll(lat,1,axis=

        M=0
        E=0

        ! total magnetization
        do x=1,20
            do y=1,20
                M=M+lat(x,y)
                E=E-1*lat(x,y)*(lat(merge(20,x-1,x<2),y)+lat(merge(1,x+1,x>19),y)+lat(x,m
            enddo
        enddo
        Etot=0
```

```
        Mtot=0

        do i=1,nmc ! Monte Carlo loop
            do j=1,400 ! Metropolis loop
                ! choose random pos
                x=floor(drand48()*20)+1
                y=floor(drand48()*20)+1
                ! check energy
                temp_e=-1*lat(x,y)*(lat(merge(20,x-1,x<2),y)+lat(merge(1,x+1,x>19),y)+lat
                dE=-2*temp_e
                if (dE.lt.0 .or. drand48().le.exp(-dE/T)) then
                    ! flip
                    lat(x,y)=-lat(x,y)
                    ! update E, M
                    E=E+2*dE
                    M=M+2*lat(x,y)
                endif
            enddo
            Etot=Etot+E/2.0
            Mtot=Mtot+M
        enddo
        E_avg=Etot*norm
        M_avg=Mtot*norm;
        print *, E,E_avg,M,M_avg,T
    enddo
end program

```

Result







The Curry temperature is around $2.2J/k_B$

Above the critical temperature, the spontaneous magnetization vanishes as the thermo effect surpass the ferromagnetic state.

From the first image, we can see the total Magnetization drops as the temperature increases. The theromo fluctuation of temperature increase starts to destroy the configuration. After reaching the critical temperature, the configuration is totally randomized, thus there is no preferred magnetic direction. Correspondingly, we can see the total energy from the second image increases as the temperature goes up.