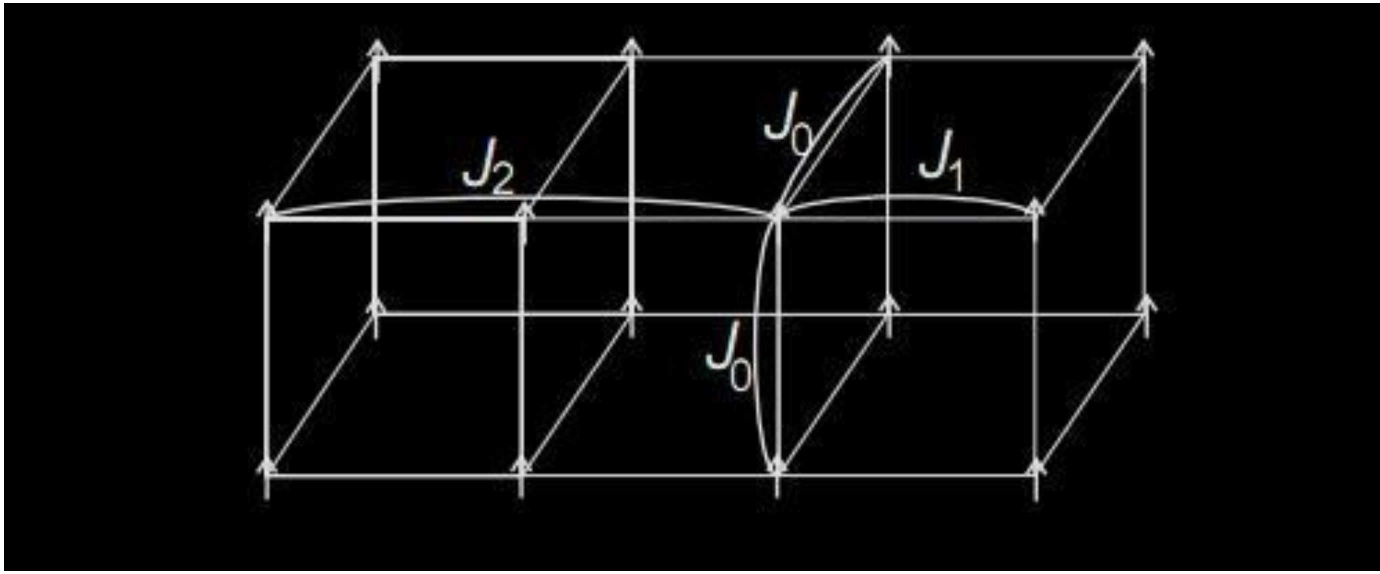


Implementing 3D ANNNI model on GPUs

Final term project – B649, Fall 2012

Dhande Nakul
Joshi Harshad

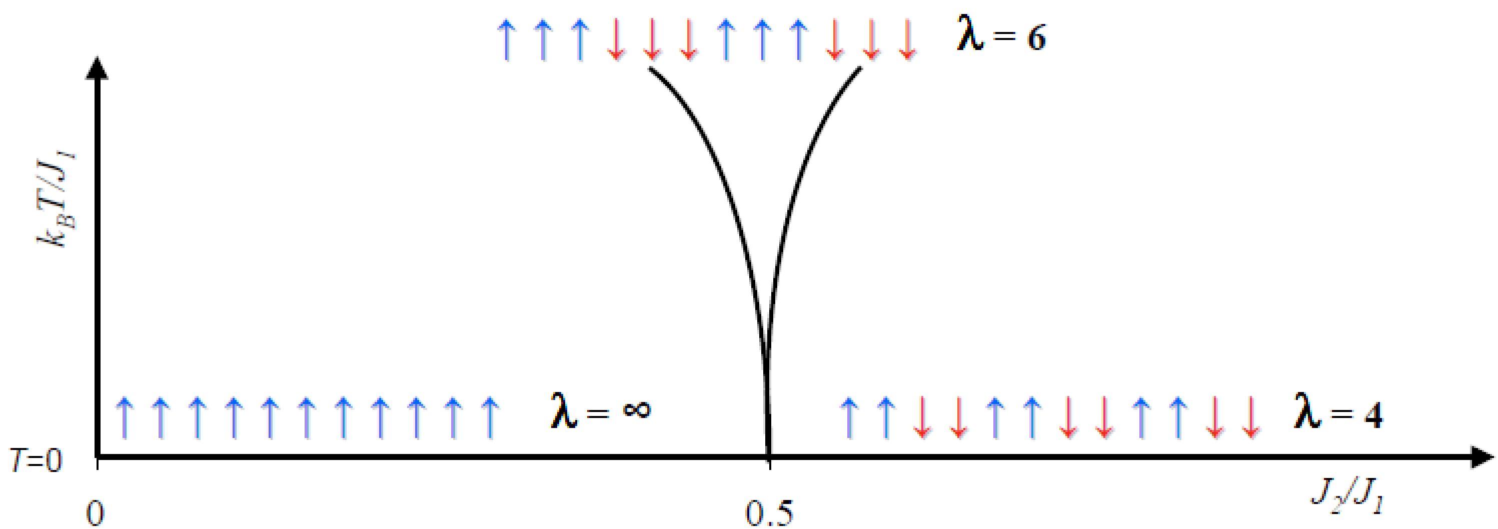
- The axial (or anisotropic) next-nearest-neighbor Ising model, or ANNNI model, is a variant of the Ising model.
- In ANNNI competing ferromagneticc and antiferromagnetic exchange interactions couple spins at nearest and next-nearest neighbor sites along one of the crystallographic axes of the lattice.
- The model is a prototype for complicated spatially modulated magnetic superstructures in crystals.
- The model was introduced in 1961 and provides a theoretical basis for understanding numerous experimental observations on commensurate and incommensurate structures, as well as accompanying phase transitions, in magnets, alloys, and other solids.
- In CSE, the most practical application is in understanding memory materials.

• ***Axial Next-Nearest-Neighbor Ising (ANNNI) model with Hamiltonian***

$$H = -J_1 \sum_{\{i,j,k\}} (\sigma_{i,j,k}\sigma_{i+1,j,k} + \sigma_{i,j,k}\sigma_{i,j+1,k} + \sigma_{i,j,k}\sigma_{i,j,k+1}) + J_2 \sum_{\{i,j,k\}} \sigma_{i,j,k}\sigma_{i+2,j,k}$$

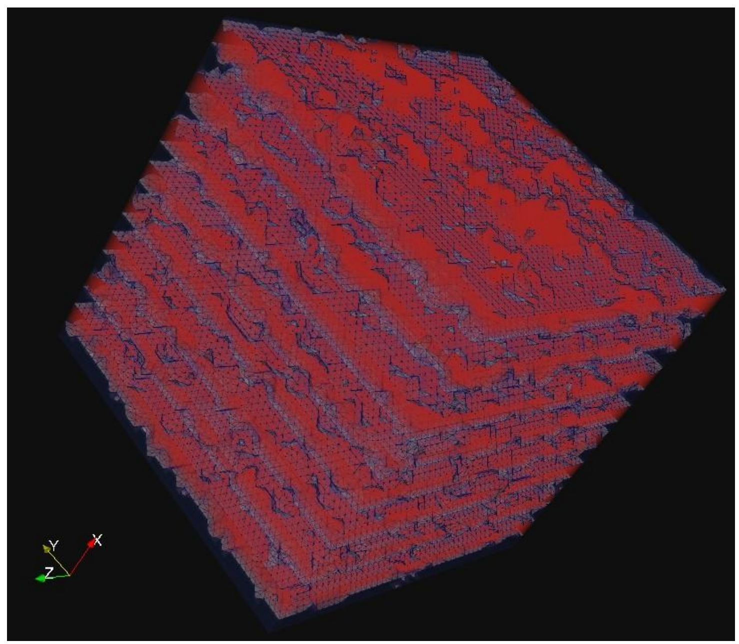
Known features of the ANNNI model at T=0

- *Ferromagnetic structure* $\uparrow\uparrow\uparrow\uparrow$ *for* $J_2/J_1 < 0.5$
- *Anti-phase structure* $\uparrow\uparrow\downarrow\downarrow$ *for* $J_2/J_1 > 0.5$
- *A highly degenerated spin structure for* $J_2/J_1 = 0.5$ *consists of successive* $\uparrow$ *and* $\downarrow$ *domains separated by walls perpendicular to the direction of competing interactions (an infinity of commensurate phases is possible)*



Notations: wavelength λ *with corresponding wave vector* $q = \dfrac{2\pi}{\lambda}$

- *Ferromagnetic phase* ↑↑↑↑↑↑↑↑↑↑↑↑ λ=∞
- *Anti-phase structure* ↑↑↓↓↑↑↓↓↑↑↓↓ λ=4 or **<2>**
- *Commensurate phase* ↑↑↑↓↓↓↑↑↑↓↓↓ λ=6 or **<3>**



Monte Carlo Methods

- Monte Carlo Casino
- Relates to use of Random Numbers
- MC or sometimes MCMC (Markov Chain Monte Carlo) methods used in variety of simulations

Ising spins: Metropolis update

$\Delta H(S,S') = H(S')-H(S)$

$$w(\underline{S} \rightarrow \underline{S}') = \begin{cases} 1 & \text{for} \quad \Delta H(\underline{S},\underline{S}') \leq 0 \\ e^{-\beta \Delta H(\underline{S},\underline{S}')} & \text{for} \quad \Delta H(\underline{S},\underline{S}') > 0 \end{cases}$$

Procedure Ising Metropolis:

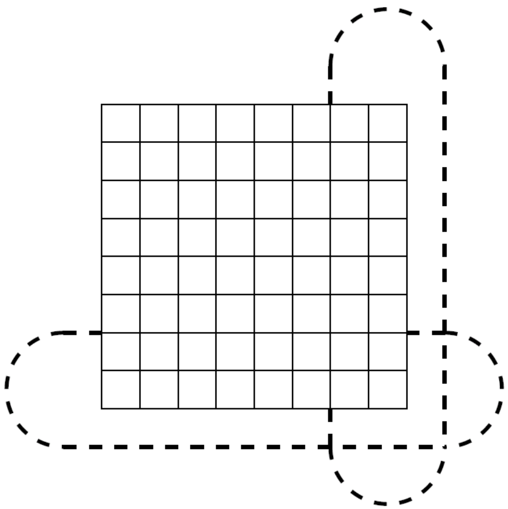
```
        Initialize S = (S_1,…,S_N)
label   Generate new configuration S‘
        Calculate ΔH= ΔH(S,S‘)
        if ΔH ≤ 0
           accept S‘  (i.e. S‘→S)
        else
           generate random numer x∈[0,1]
           if x<exp(-βΔH)
               accept S‘  (i.e. S‘→S)
        compute O(S)
        goto label
```

Single spin flip Metropolis for Ising

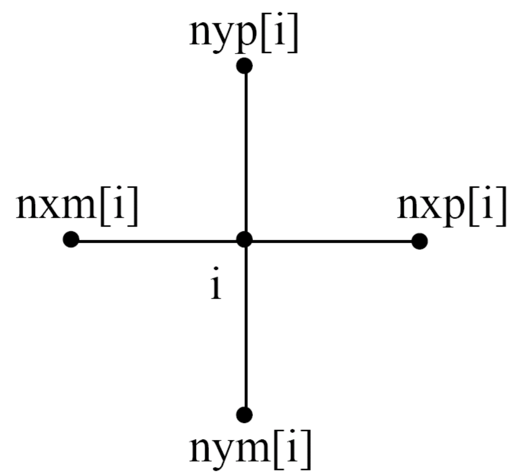
```
Procedure single spin flip
  Input L,T, N=L*L
  Define arrays: S[i], i=1,…,N, h[i], i=1,…,N, etc.
  Initialize S[i], nxm[i], nxp[i],…., h[i]
  step = 0

  while (step<max_step)
     choose random site i
     calculate dE = 2*h[i]*S[i]
     if ( dE <= 0 )
         S[i]=-S[i]; update h[nxm[i]], h[nxp[i]],…
     else
        p = exp(-dE/T)
        x = rand()
        if ( x<p)
          S[i]=-S[i]; update h[nxm[i]], h[nxp[i]],…
     compute M(S), E(S), …
     accumulate M, E, …
     step++
  Output m, e, …
```

Implementation issues

Periodic boundary conditions



Neighbor tables



e.g.: $\text{nxp}[i] = i+1$ if $i\%L \neq 0$

$= i+1-L$ if $i\%L = 0$ etc.

Random number generation

- Pseudo random number generators
- Why we cannot use rand() function
  - Not thread safe
  - Depends on a shared state for random number generation.
- Random 123

Random number generation

- Random123:
  - Long period
  - Counter based
  - Can produce at least 2^{64} unique parallel streams
  - Period of 2^{128} or more.
  - Philox PNRG is faster than CURAND library on single NVIDIA GPU.

Parallelizing ANNNI

- Multi-threaded implementation
  - Optimizations:
    - Cache optimization techniques by analyzing the loop structure of ANNNI algorithm
    - Loop parallelization
- ANNNI on GPU
  - Challenges:
    - Maximize the part of code to be run in parallel on GPU.
    - Program correctness.

References

- D. E. Shaw's paper on "Random123" http://www.thesalmons.org/john/random123/papers/random123sc11.pdf

Thank You!