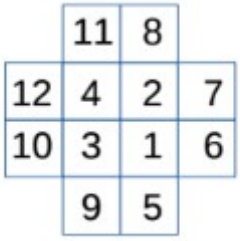
The system consists of a square lattice of nc columns and nr rows, with lattice points (e.g. for a 100x100 lattice) numbered as

901	902	903	…	1000
...	...	...	...	...
...	...	...	...	...
101	102	103	…	200
1	2	3	…	100

The proteins consist of 12 lattice points and they are labelled as follows:



In the manuscript each lattice point can take a value of -1, -0.5, 0, 0.5, or 1. However, in our code we use spin values ranging from 0 to 1. These two conventions can be made equivalent with the following substitutions:

0 → -1
0.25→ -0.5
0.5→ 0
0.75 → 0.5
1 → 1

COMPILING THE CODE

gfortran -fdefault-real-8 common.f90 routines.f90 main.f90 -o run.exe

INPUT FILES

- ising.inp

  This file requires the following structure:

  ```
  nx      ny      nmove
  temp    inter   frac    init    thermo          seed
  eq      prod    freq    write
  ```

  nx: number of rows
  ny: number of columns
  nmove: number of attemps for swapping a spin in each Monte Carlo cycle
  temp: temperature of the system in 1/kB units
  inter: J parameter in the Ising Model in J/kBT units
  frac: Fraction of lattice points with spin +1. Only relevant if starting a new configuration.

init: Determines if a new configuration is started.
0 → No
1 → Yes
If the option 0 is set, a file spins.txt with the spin values of the old configuration is needed. This file must contain each spin value in a different row.
thermo: Set to 1.
seed: random number of 9 digits for the random number generator
eq: number of equilibration cycles
prod: number of production cycles
freq: frequency (in number of MC cycles) to collect data
write: determines if the intermediate configurations are written in a file named raw_spins.dat. This is a binary file, where the first row contains the number of configurations and number of lattice points. The following rows contain the spin values of each lattice point for all the configurations written one after each other.
0 → No
1 → Yes

- interactions.inp

  This file requires the following structure:

  inter size init dist
  sblock1 sblock2
  ilambda ext
  pattern
  nlat

  inter: determines the number of proteins present in the system
  1 → one protein growing in the lipid matrix (state β)
  3 → one protein growing in a matrix where a protein is already present (state δ grown from β)
  size → set to 4
  init: number of the lattice point where position 1 of the first protein is located
  dist: distance (in lattice points) between positions 1 of the first and second proteins
  sblock1: target spin value of protein 1. Only applies if the protein is homogeneous
  sblock2: target spin value of protein 2. Only applies if the protein is homogeneous
  ilambda: value of the parameter lambda in the thermodynamic integration
  ext: strength of the external field in kBT units
  pattern: determines if the protein is homogeneous
  0 → homogeneous
  1 → non homogeneous
  If the option 1 is set, the files spins1.dat and spins2.dat are requiered. This files must contain the target spin values of proteins 1 and 2 (one spin value in each row), respectively, labelled according to the sketch shown above.
  nlat: number of lattice points in a row

OUTPUT FILES

- spins.txt: file with the final configuration
- instant_ener.xyz: this file contains the total energy of the system at different points of the simulation. The first column contains the MC cycle and the second column the total energy

- ener_ti.dat: this file has two columns. The first one is the MC cycle, and the second one corresponds to the instant values of H_{fin}-H_{ini} with which the average value of the integrand in eq.7 of the manuscript can be computed.
- av_spins_surroundings.dat. File with the average spins of each lattice point at the end of the simulation.