



Workshop: Magnets Problem

Adám Brudzewsky

Richard Park

Rodrigo Girão Serrão



Workshop Overview

- ◆ Day 1: TotalEnergy
 - a. Algorithms
 - b. Writing general code
 - c. Exercises
- ◆ Day 2: Simulate
 - a. Code Review
 - b. Performance Tuning
 - c. Exercises



TotalEnergy

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

$$W \quad \begin{matrix} N \\ \textcolor{brown}{S} \\ S \end{matrix} \quad E$$

$$\textcolor{brown}{S}_E = -J \times \textcolor{brown}{S} \times (N + E + S + W)$$



TotalEnergy using Stencil

$$\begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 & 1 \\ -1 & -1 \\ 1 & -1 \\ -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$



TotalEnergy using Stencil

$$\begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 & 1 \\ -1 & -1 \\ 1 & -1 \\ -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



TotalEnergy using Shifting

$$\begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 & 1 \\ -1 & -1 \\ 1 & -1 \end{matrix}$$
$$\begin{matrix} -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$



TotalEnergy using Shifting

$$\begin{array}{ccccc} 0 & \left[\begin{array}{ccc} -1 & -1 & 1 \end{array} \right] & -1 \\ 0 & \left(\begin{array}{ccc} 1 & -1 & 1 \end{array} \right) & -1 \\ 0 & \left[\begin{array}{ccc} 1 & 1 & -1 \end{array} \right] & 1 \\ 0 & \begin{array}{ccc} -1 & 1 & 1 \end{array} & 1 \\ 0 & \begin{array}{ccc} 1 & -1 & -1 \end{array} & -1 \end{array}$$



TotalEnergy using Shifting

$$\begin{bmatrix} -1 & -1 & 1 \\ \textcircled{1} & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 \\ -1 \\ 1 \end{matrix}$$
$$\begin{matrix} -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \end{matrix}$$



TotalEnergy using Shifting

$$\begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 & 1 \\ -1 & -1 \\ 1 & -1 \end{matrix}$$
$$\begin{matrix} -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$



TotalEnergy using Shifting

$$\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ \left[\begin{array}{ccc} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{array} \right] & -1 & 1 \\ & -1 & -1 \\ & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 \end{array}$$



TotalEnergy using Shifting

$$\begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \begin{matrix} -1 & 1 \\ -1 & -1 \\ 1 & -1 \end{matrix}$$
$$\begin{matrix} -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$



TotalEnergy using N-wise Reduce

-1	-1	1	-1	1
1	-1	1	-1	-1
1	1	-1	1	-1
-1	1	1	1	1
1	-1	-1	-1	1



TotalEnergy using N-wise Reduce

-1	-1	1	-1	1
1	× -1	1	-1	-1
1	1	-1	1	-1
-1	1	1	1	1
1	-1	-1	-1	1



TotalEnergy using N-wise Reduce

-1	-1	1	-1	1
1	× -1	1	-1	-1
1	1	-1	1	-1
-1	1	1	1	1
1	-1	-1	-1	1



TotalEnergy using N-wise Reduce

-1	-11	-11	-11
-11	-11	-11	-1
1	-11	-11	-11
-11	1	1	1
-11	-1	-1	-11



TotalEnergy using N-wise Reduce

1	-1	-1	-1
-1	-1	-1	1
1	-1	-1	-1
-1	1	1	1
-1	1	1	-1



TotalEnergy using N-wise Reduce

0	1	-1	-1	-1
0	-1	-1	-1	1
0	1	-1	-1	-1
0	-1	1	1	1
0	-1	1	1	-1



Break



Maintainability

- Others (and our future selves) can easily understand our code
Code is read much more often than it is written, so plan accordingly
- It is easy to make changes to the behaviour



Changing the Rules

- Change "constants"
 - Interaction constant
 - Temperature
- Add an external magnetic field



Changing the Rules

- Which neighbours
 - Nearest neighbours
 - Anisotropic influence
 - Distant neighbours



Changing the Rules

- World shape
 - Plane
 - Cylinder
 - Torus



Interaction Constant

$$E = \textcircled{-J} \sum_{ij} s_i s_j$$



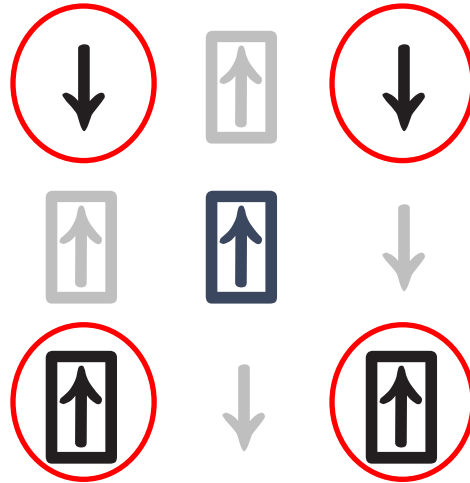
External Field

$$E = -J \sum_{ij} s_i s_j - h \sum_j s_j$$



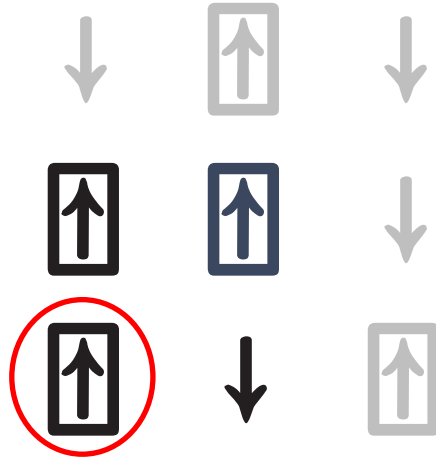
Change contribution from neighbours

- Corners also contribute



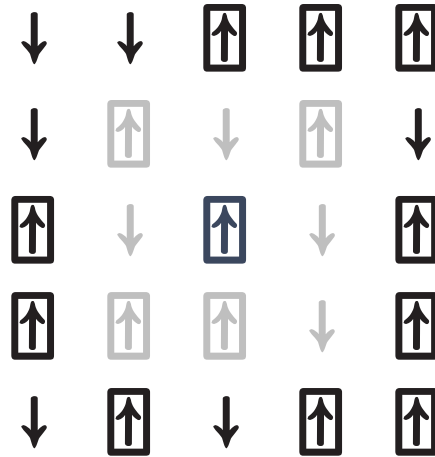
Change contribution from neighbours

- Anisotropic: southwest neighbours contribute more



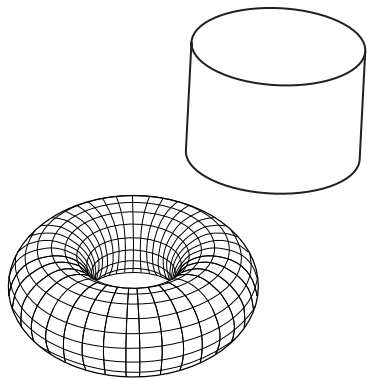
Change contribution from neighbours

- More distant neighbours contribute more than nearby neighbours



Change the World Shape

- ✧ Bounded plane
From the problem description, we do not flip edge spins
- ✧ Cylinder: one edge wraps around
- ✧ Torus: all edges wrap around
- ✧ **BONUS:** Consider
 - ✧ Non-rectangular lattice
 - ✧ 3D (or higher?)



Exercise

Choose one of the approaches we discussed and implement it to be easy to adjust for as many of the rule changes as you can

- ✧ Production quality code
- ✧ Sensible variable names
- ✧ Comments

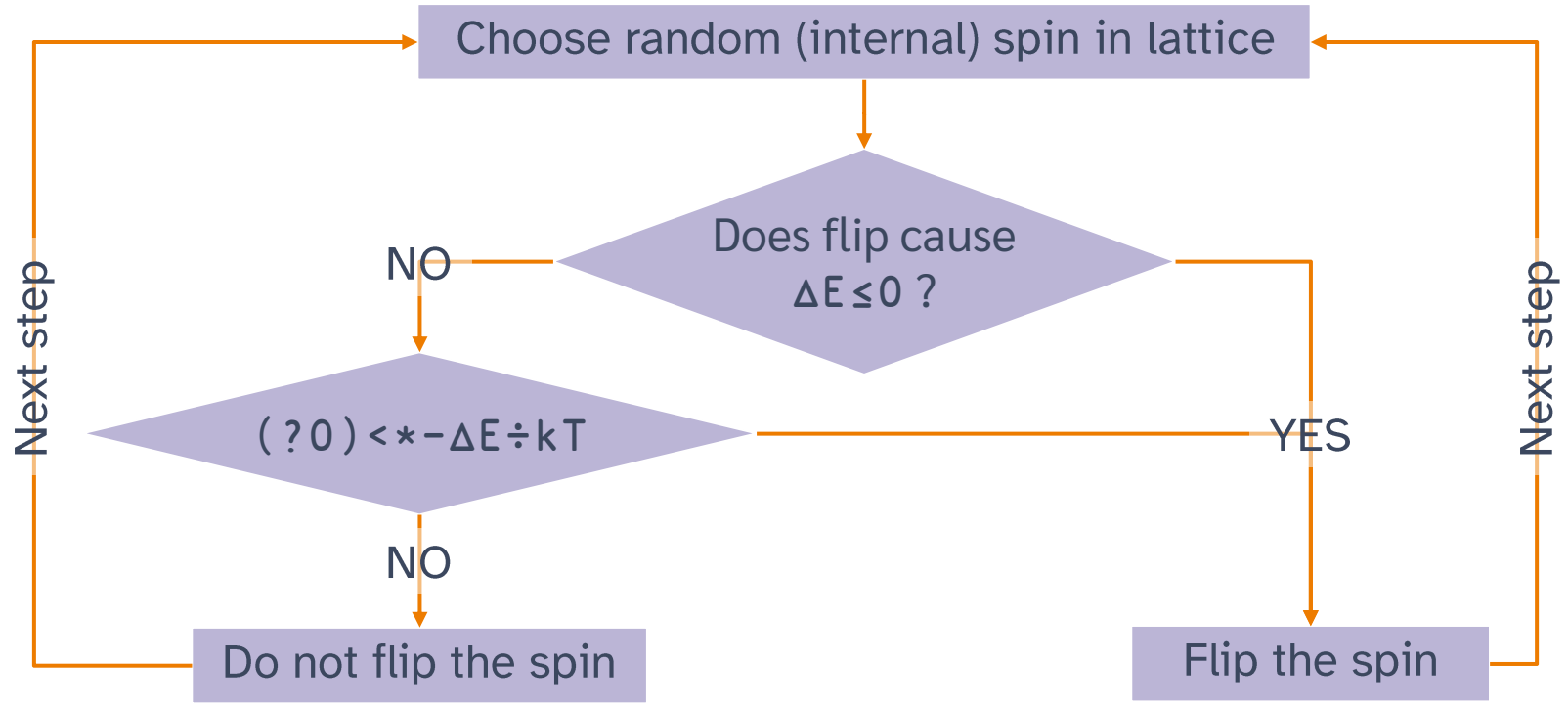


See you next week!

🟡 Questions?



Simulate: The Metropolis Algorithm



Code Review

This code supposedly chooses a random spin to flip.

```
shape ← plat  
random ← ?shape  
random -← random=shape  
random +← random=1
```

- Can you spot the mistake?



Code Review

This code supposedly chooses a random spin to flip.

```
random ← 1+2-2+lat
```

- Can you spot the mistake?



Code Review

This code supposedly chooses a random spin to flip, then does it or not, depending on DoFlip ΔE .

- Can you spot the mistake?

```
RandomFlip  $\leftarrow$   $\{-\text{@}(1+\text{?}^{-2}+\rho\omega)\vdash\omega\}$   
 $\Delta E \leftarrow (\text{TotalEnergy RandomFlip lat}) - \text{TotalEnergy lat}$   
:If DoFlip  $\Delta E$   
    lat  $\leftarrow$  RandomFlip lat  
:EndIf
```



Code Review: Bonus

This code supposedly chooses all random spins to flip, for the entire simulation, at once.

- Can you spot the mistake?

```
shape←p1at  
all_random ← 1+shape10?n 2pshape-2
```



How to detect / prevent errors?

- ✧ Simple visualisation
- ✧ Logging
- ✧ Plotting

