

Development of a Graphical Interface for Monte Carlo Simulations of Magnetic Crystals

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The Problem

- want to understand the magnetic properties of materials
- Constructing Models and calculating spins is very tedious.
- The Goal: Create a program to simplify this process

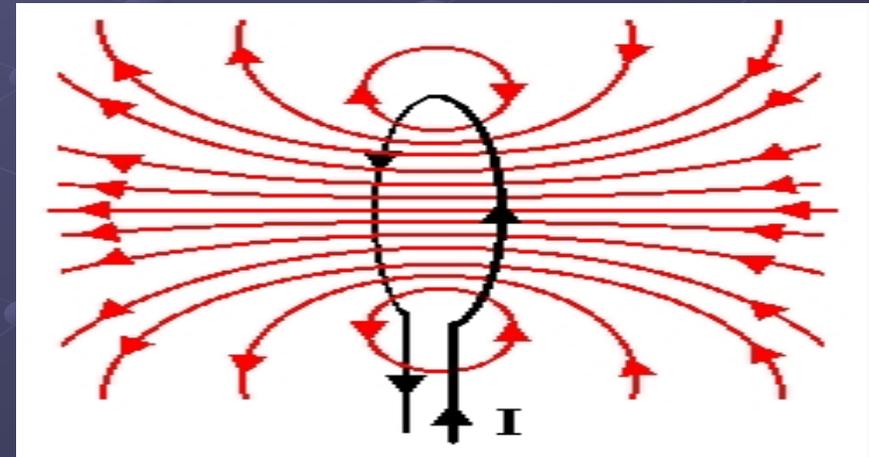
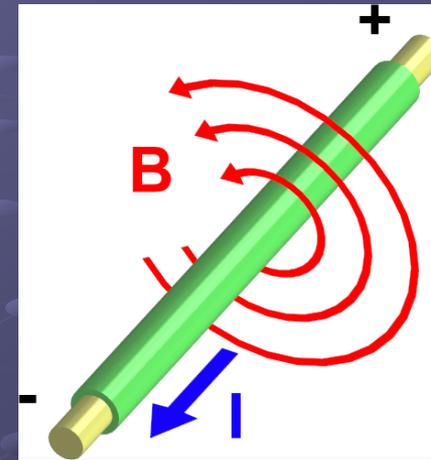
Why We Care

- Used constantly in everyday life
- Motors
- Transformers
- Hard Drives
- MRAM



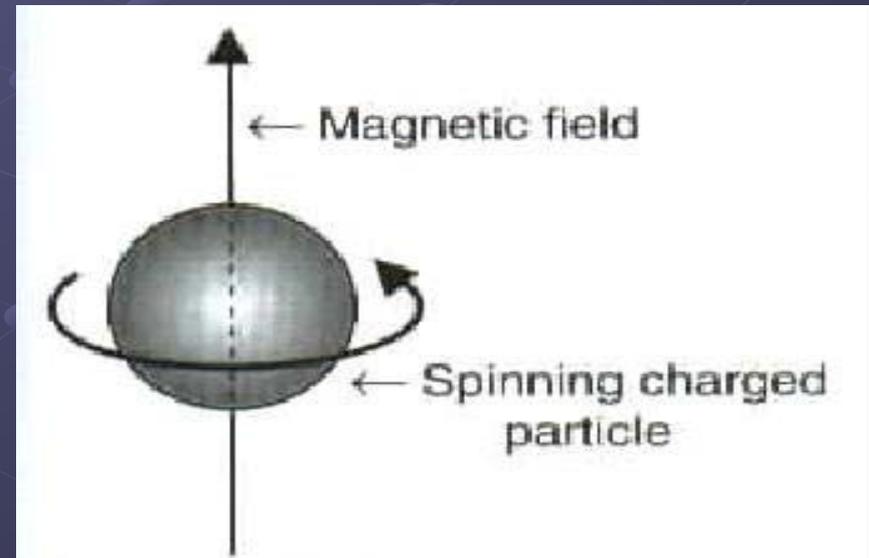
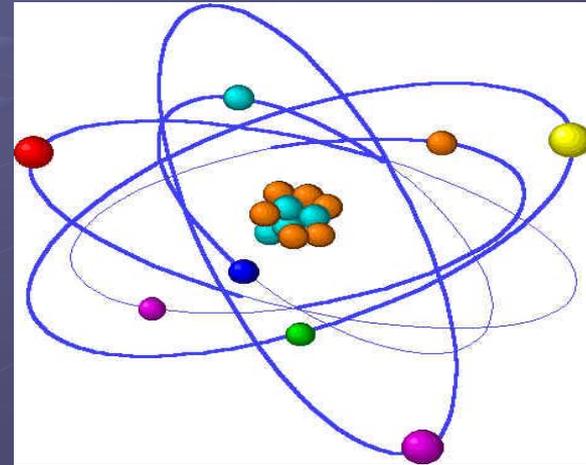
Magnetism

- Electric Current creates circular magnetic field perpendicular to current
- A current loop will create a magnetic dipole

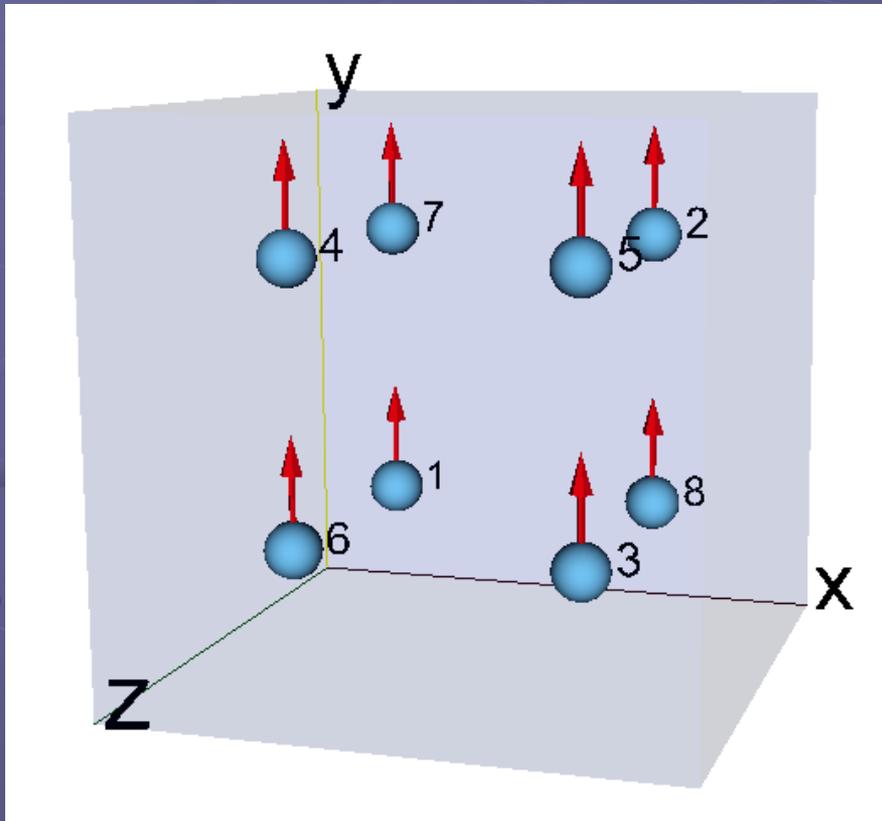


Angular Movement of Electrons

- Two kinds of angular motion within atom:
- Orbital motion-
Classical model is directly analogous to a current loop
- Spin – Intrinsic quantum mechanical property represented as a vector



Magnetic Properties of Insulators

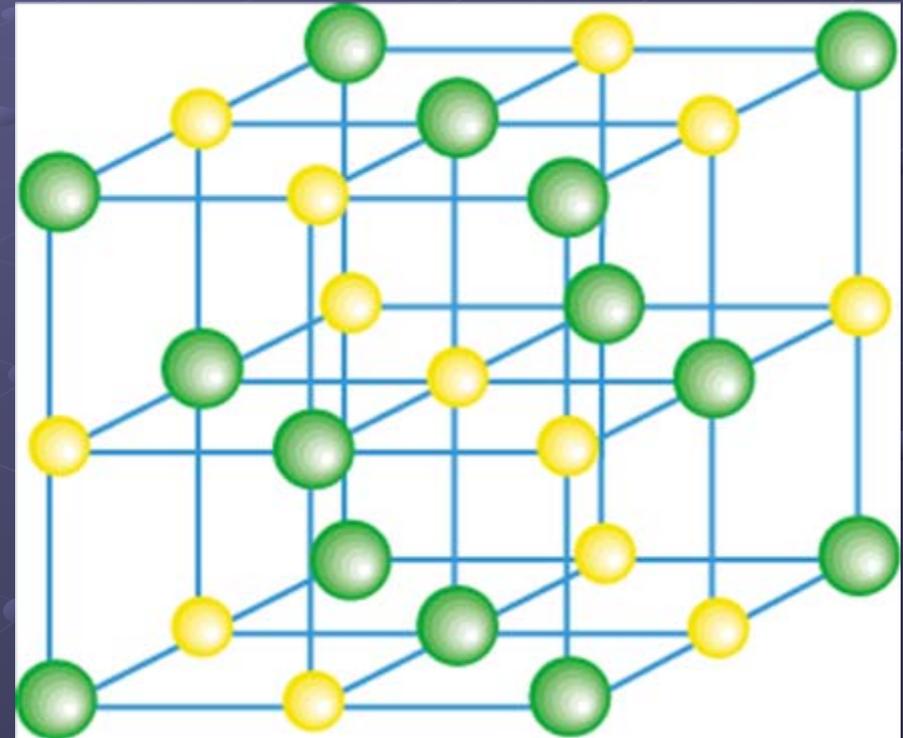


- Atoms can end up with net spins.
- Depending on interactions, Spins tend to align in certain ways, i.e. Ferromagnetic, anti-ferromagnetic, etc.



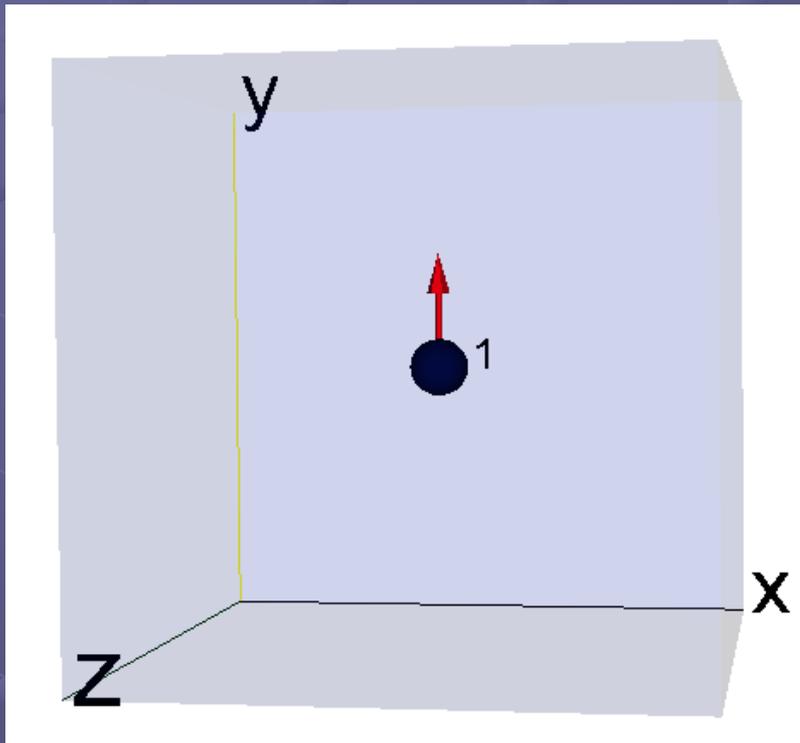
Lattice Structure

- Regular, repeating arrangement of atoms.
- The smallest unique group of atoms is called the unit cell.
- Unit cell translates to form whole lattice
- Similarly, the magnetic unit cell, is the smallest unique arrangement of atoms and their spins.

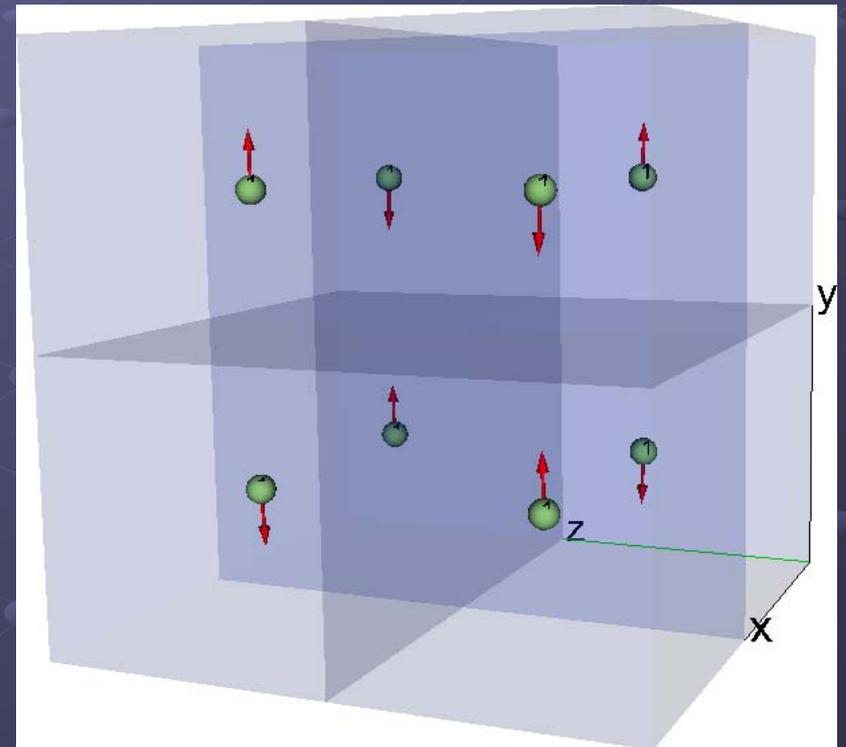


Example

- Crystallographic Unit Cell

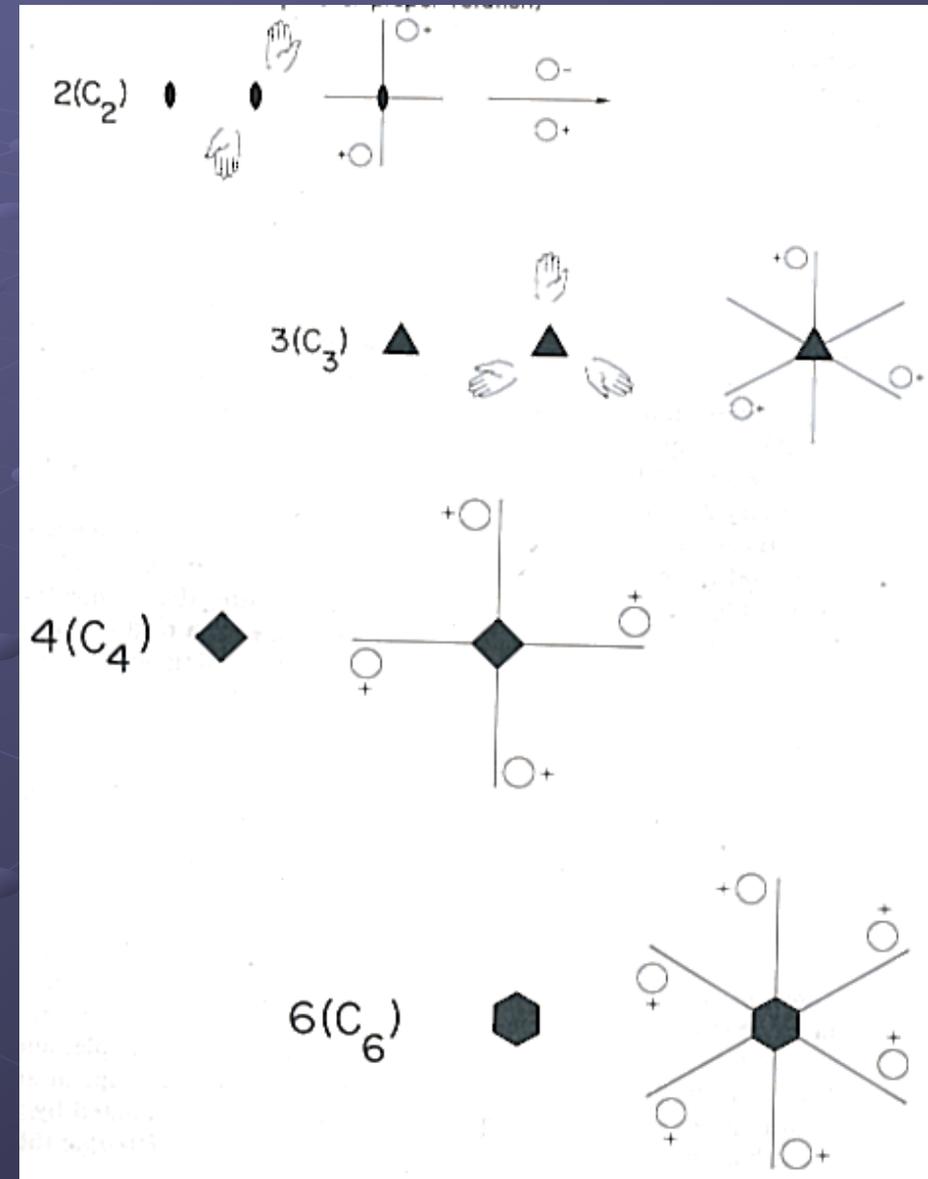


- Magnetic Unit Cell



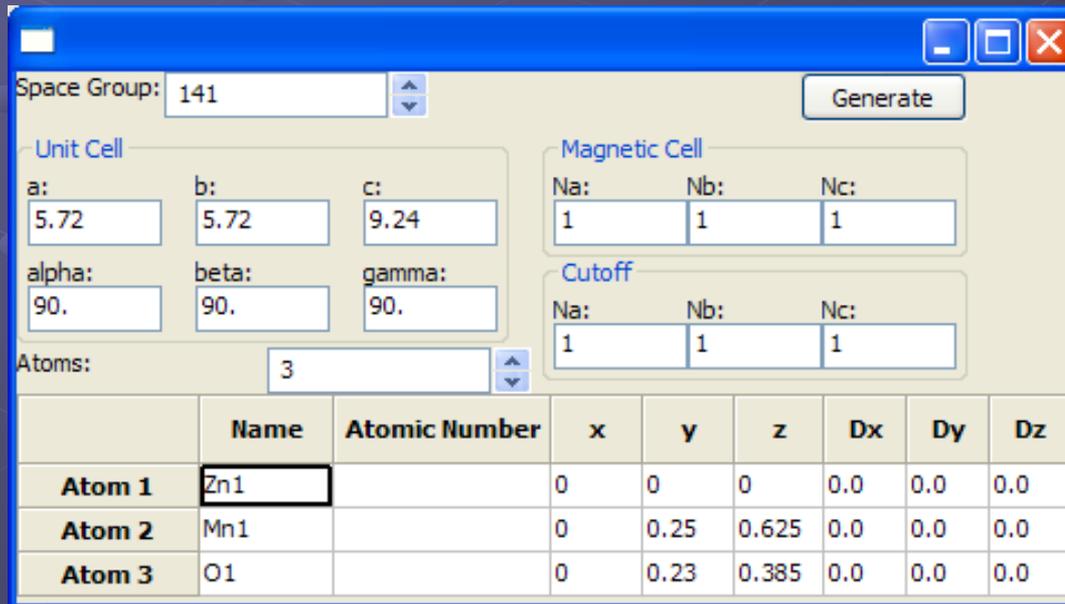
Space Groups

- Mathematical symmetry operations; i.e.. rotations, reflections, etc.
- 230 space groups.
- Any crystal lattice can be represented by a space group.



The Program: Atoms

- The user enters the space group and initial positions of 1 or more atoms in the lattice.
- Program then creates the crystallographic unit cell
- The atoms in the crystallographic unit cell are then translated to form the magnetic unit cell.



The screenshot shows a software window with the following fields and a table:

Space Group: 141 Generate

Unit Cell

a: 5.72 b: 5.72 c: 9.24

alpha: 90. beta: 90. gamma: 90.

Atoms: 3

Magnetic Cell

Na: 1 Nb: 1 Nc: 1

Cutoff

Na: 1 Nb: 1 Nc: 1

	Name	Atomic Number	x	y	z	Dx	Dy	Dz
Atom 1	Zn1		0	0	0	0.0	0.0	0.0
Atom 2	Mn1		0	0.25	0.625	0.0	0.0	0.0
Atom 3	O1		0	0.23	0.385	0.0	0.0	0.0

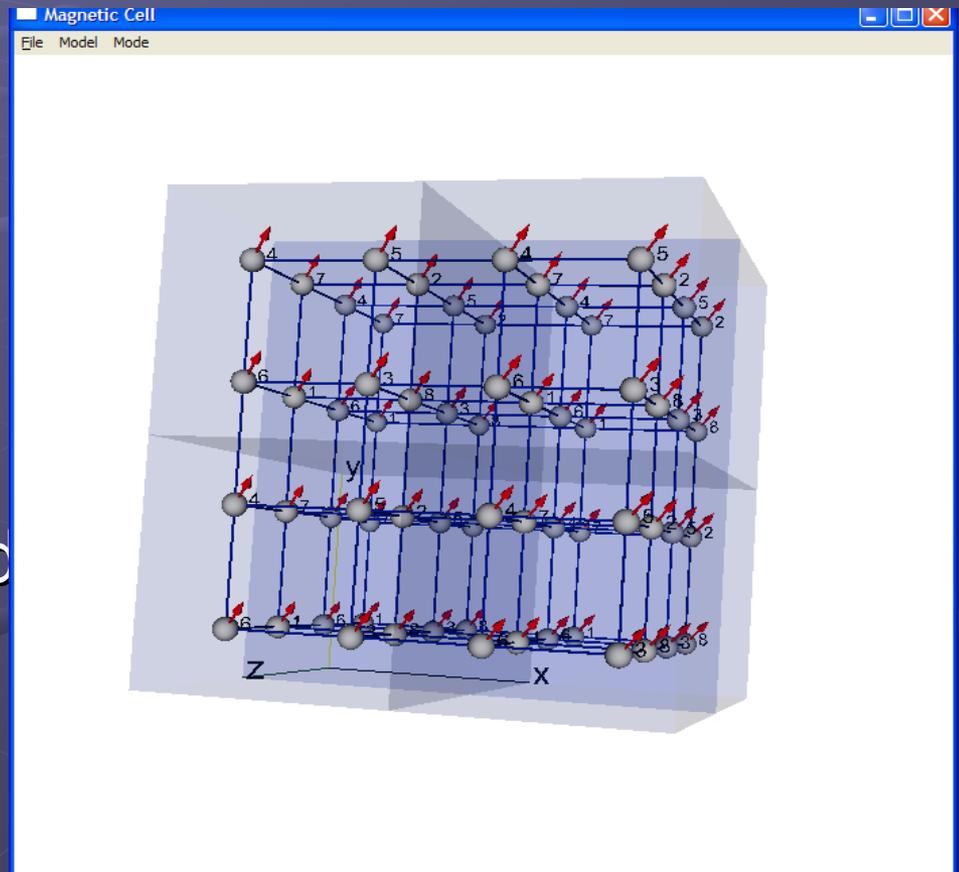
The Program: “Bonds”

Bonds										
3 <input type="button" value="Generate"/>										
	Atom1 Number	Na	Nb	Nc	Atom2 Number	Na	Nb	Nc	Jij Matrix	On
Bond 1	1	0	1	1	6	0	1	1	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X
Bond 2	4	0	1	1	6	0	1	1	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X
Bond 3	3	0	1	1	6	0	1	1	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X

- Once the atoms are created, the user can add an interaction between any two atoms.
- Along with the connected atoms, the user can enter an interaction matrix describing the interaction between the spins of the two atoms.
- The “bond” is then automatically transformed and translated throughout the magnetic cell.

The Program Continued

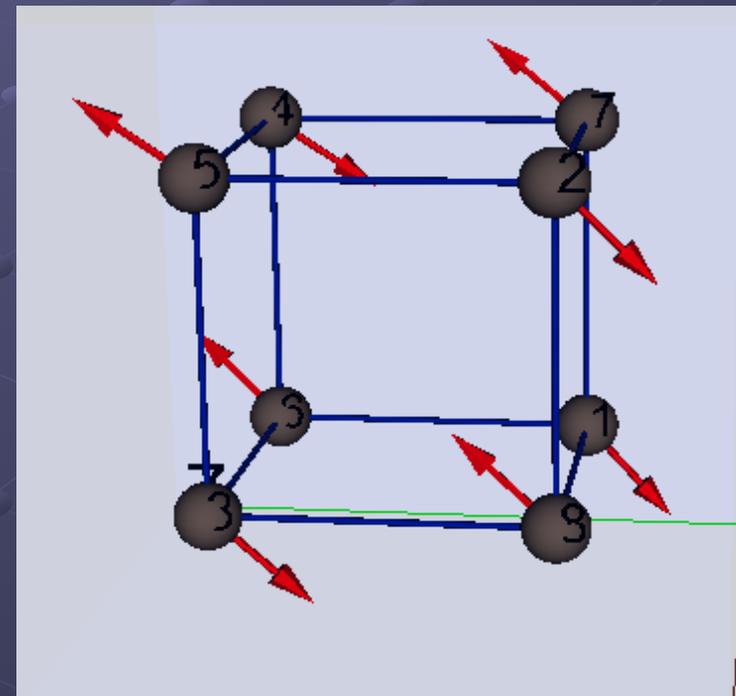
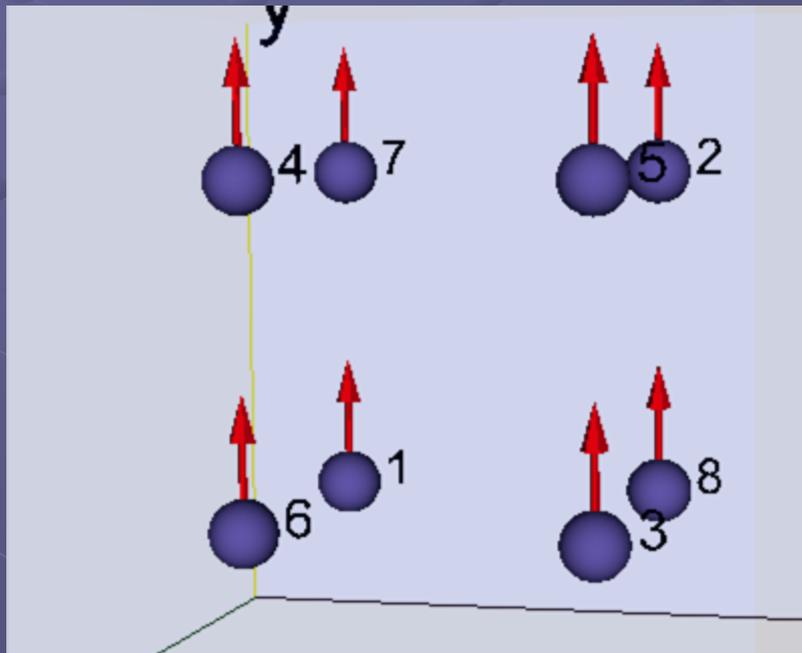
- 3D model is displayed.
- Interactions can be interactively added.
- Once atoms and “bonds” are generated, the ground state spin configuration can be found using a Monte Carlo Simulation.



Ground State

● Ferromagnetic

● Anti-ferromagnetic



Simulated Annealing

- Try to minimize energy
- That can become a very difficult calculation for large lattices, so we use a Monte Carlo Simulation.
- Monte Carlo Simulations use large numbers of random configurations to find the best.

Simulated Annealing

- Minimize Energy with random spin fluctuations:

- $$E = -S_1 J_{ij} S_2 - D_x S_{1x}^2 - D_y S_{1y}^2 - D_z S_{1z}^2$$

- Probability of a move to higher Energy:

- $$e^{-\Delta E/T}$$

Example Run

Atoms

Space Group:

Unit Cell

a: b: c:

alpha: beta: gamma:

Magnetic Cell

Na: Nb: Nc:

Atoms:

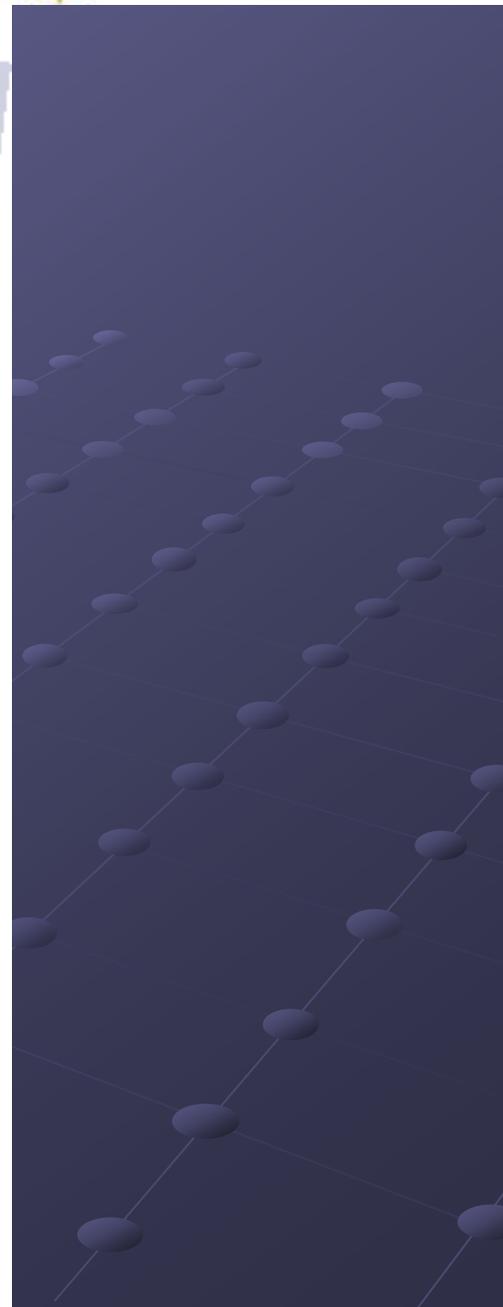
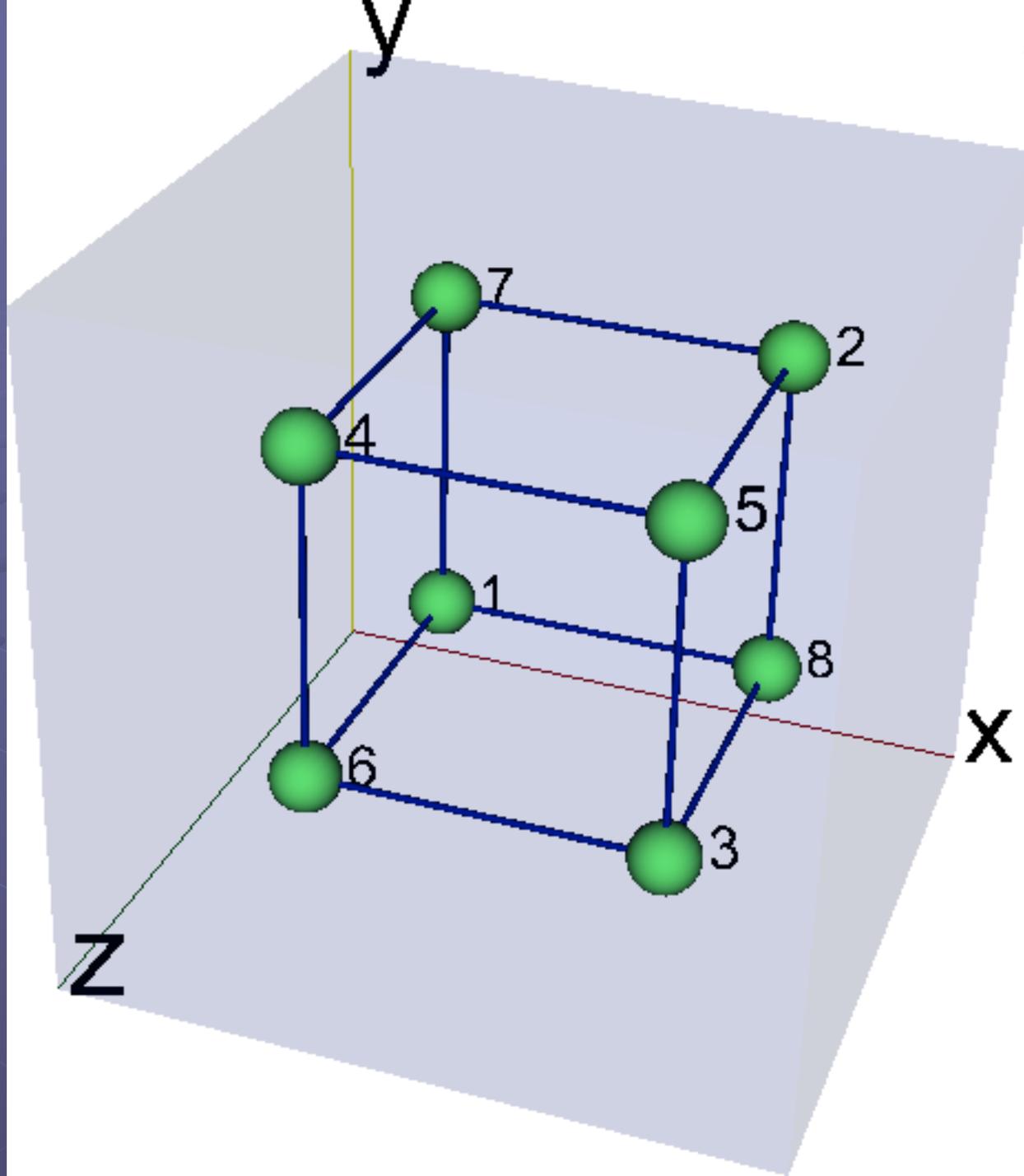
Cutoff

Na: Nb: Nc:

	Name	Atomic Number	x	y	z	Dx	Dy	Dz
Atom 1	Atom1	1	.25	.25	.25	0.0	0.0	0.0

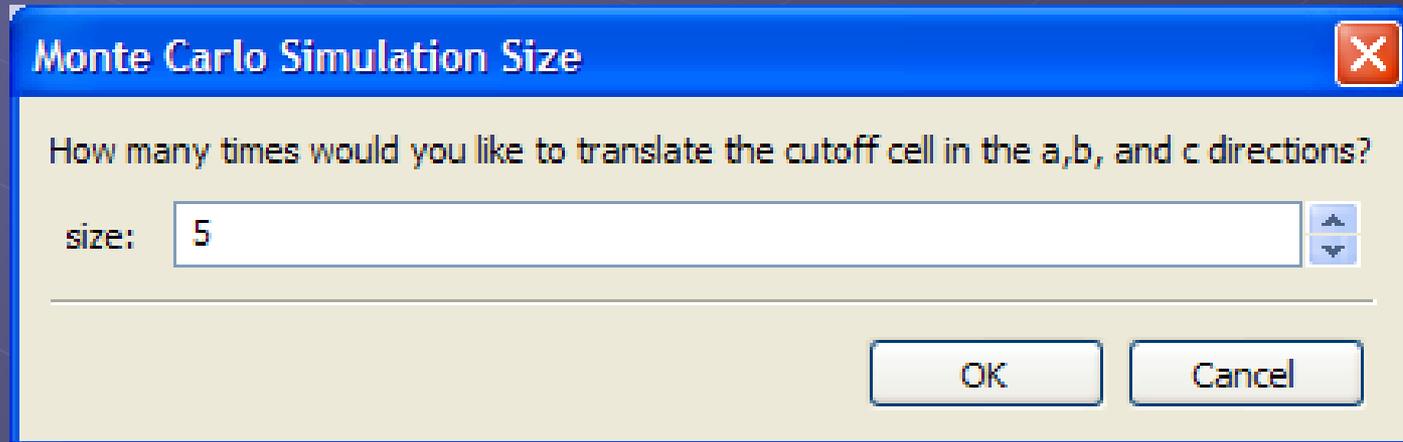
Example Run

Bonds										
3										
Generate										
	Atom1 Number	Na	Nb	Nc	Atom2 Number	Na	Nb	Nc	Jij Matrix	On
Bond 1	6	0	0	0	4	0	0	0	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X
Bond 2	4	0	0	0	5	0	0	0	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X
Bond 3	7	0	0	0	4	0	0	0	[[1. 0. 0.] [0. 1. 0.] [0. 0. 1.]]	X



Translating the Lattice

- Translate Cutoff Cell to reduce finite size effects

A screenshot of a software dialog box titled "Monte Carlo Simulation Size". The dialog box has a blue title bar with a close button (X) in the top right corner. The main area is light yellow and contains the text "How many times would you like to translate the cutoff cell in the a,b, and c directions?". Below this text is a text input field with the number "5" entered. To the left of the input field is the label "size:". At the bottom of the dialog box are two buttons: "OK" and "Cancel".

Monte Carlo Simulation Size

How many times would you like to translate the cutoff cell in the a,b, and c directions?

size: 5

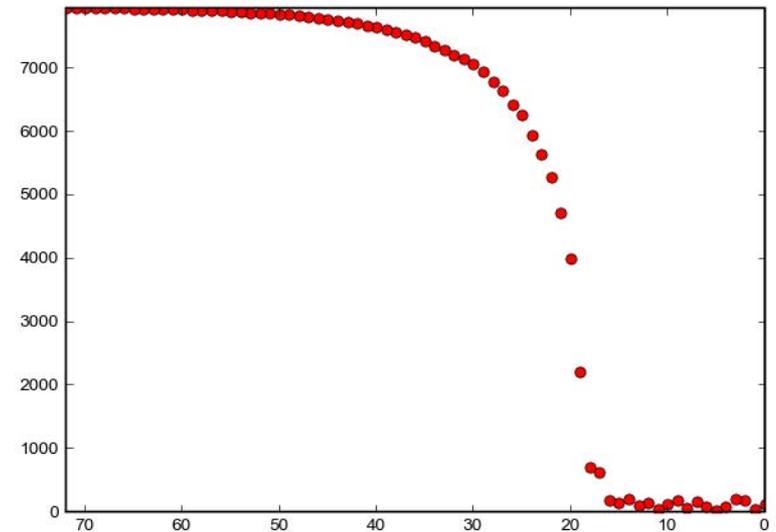
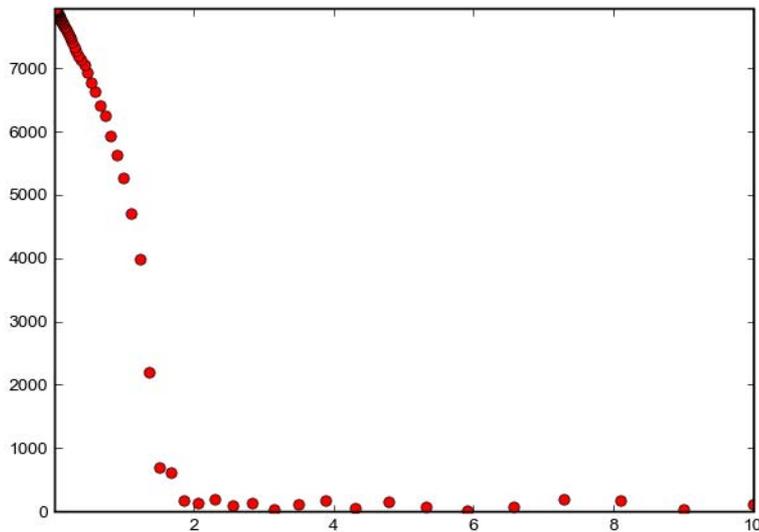
OK Cancel



Finding the Ground State

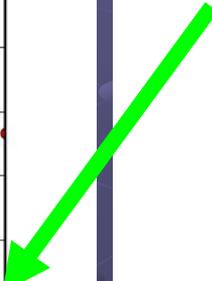
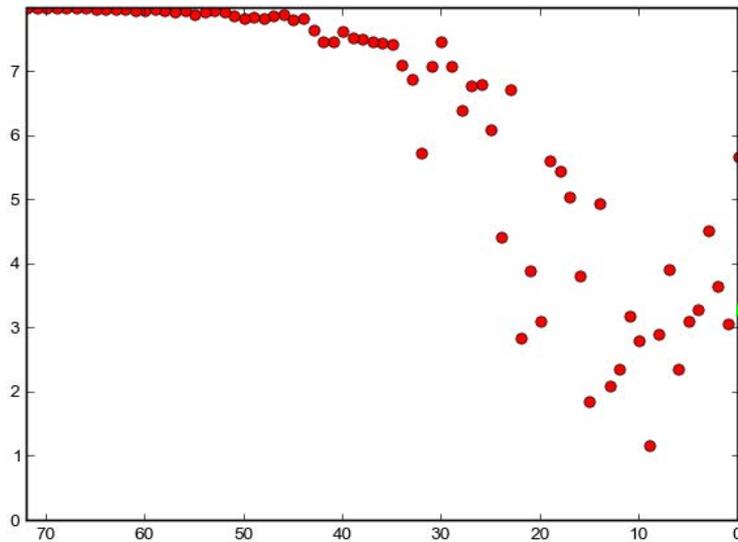
● Magnetization vs. Temperature

● Magnetization vs. Iteration Number

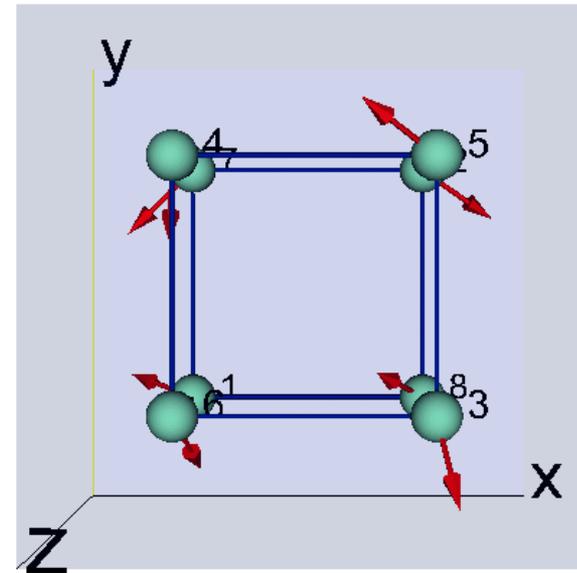


Spins at $T = 10$

● Magnetization vs. Iteration Number

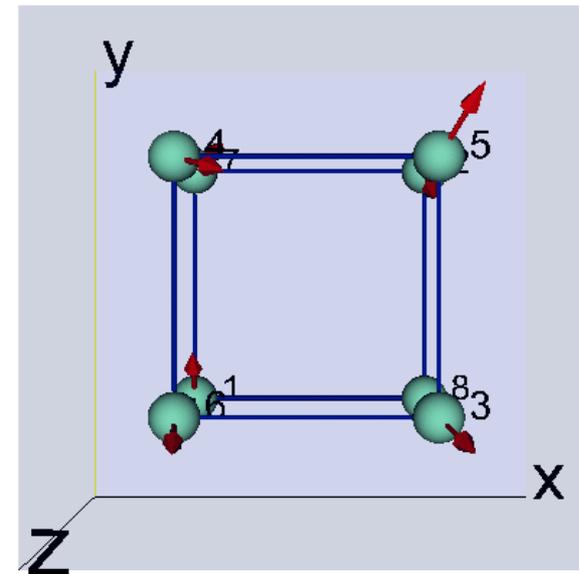
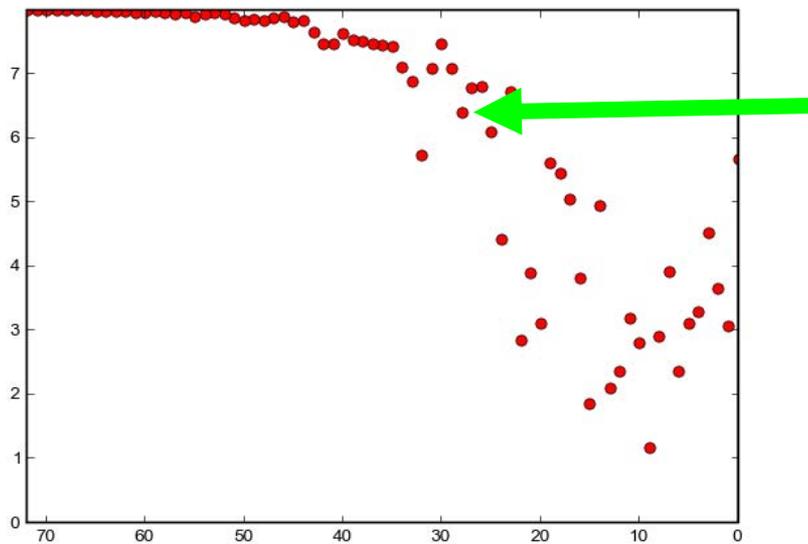


Output snapshots



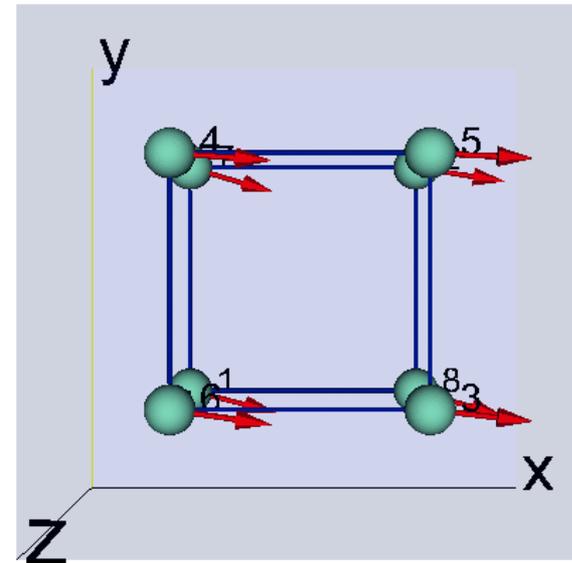
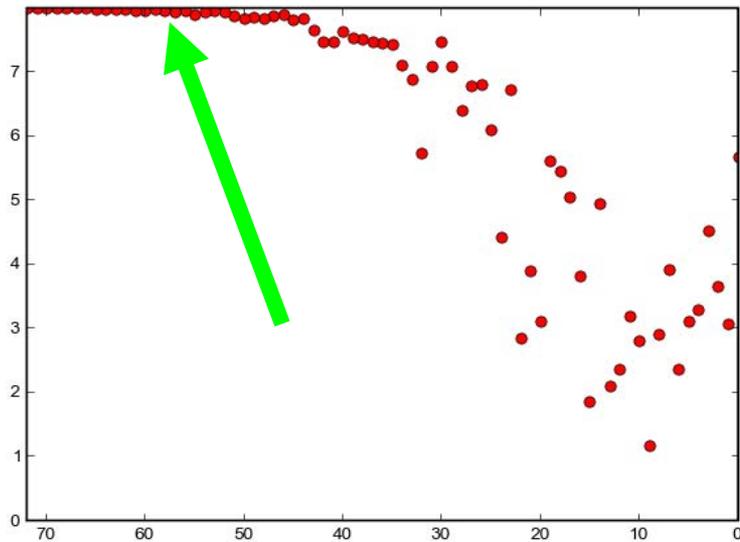
Spins at $T = .4$

- Magnetization vs. Iteration Number



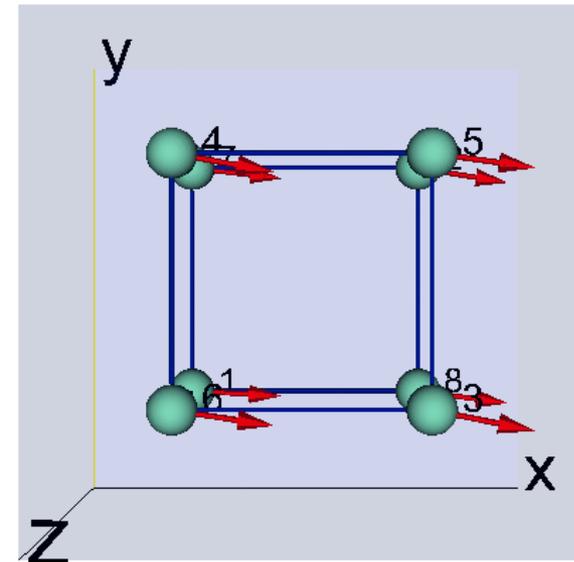
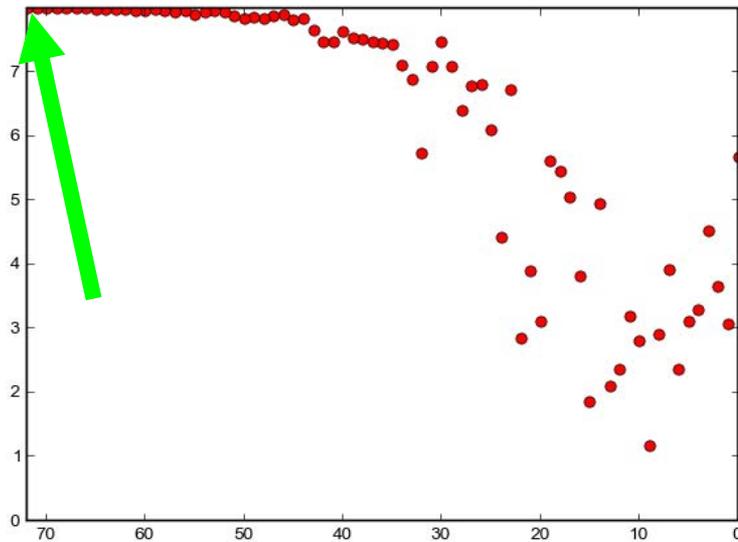
Spins at $T = .02$

- Magnetization vs. Iteration Number



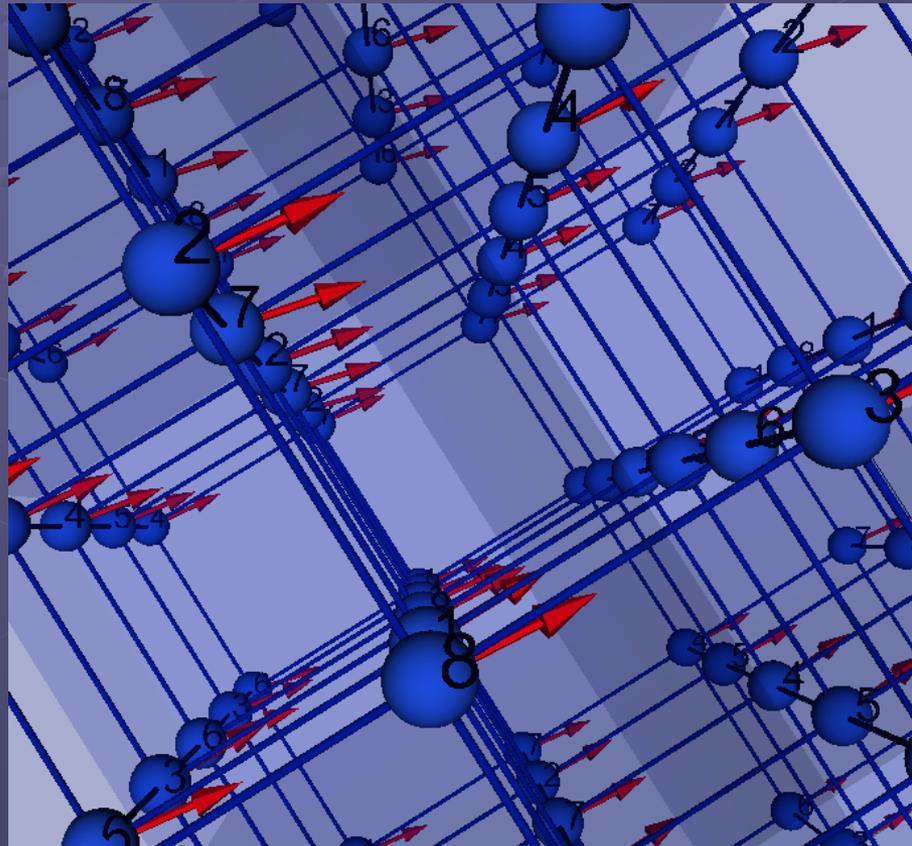
Spins at $T = .005$

- Magnetization vs. Iteration Number



The Future

- Excitations above the ground state
- Symmetry Constraints



...And it was the best summer ever

