



Spin-Interactions Using Reinforcement Learning

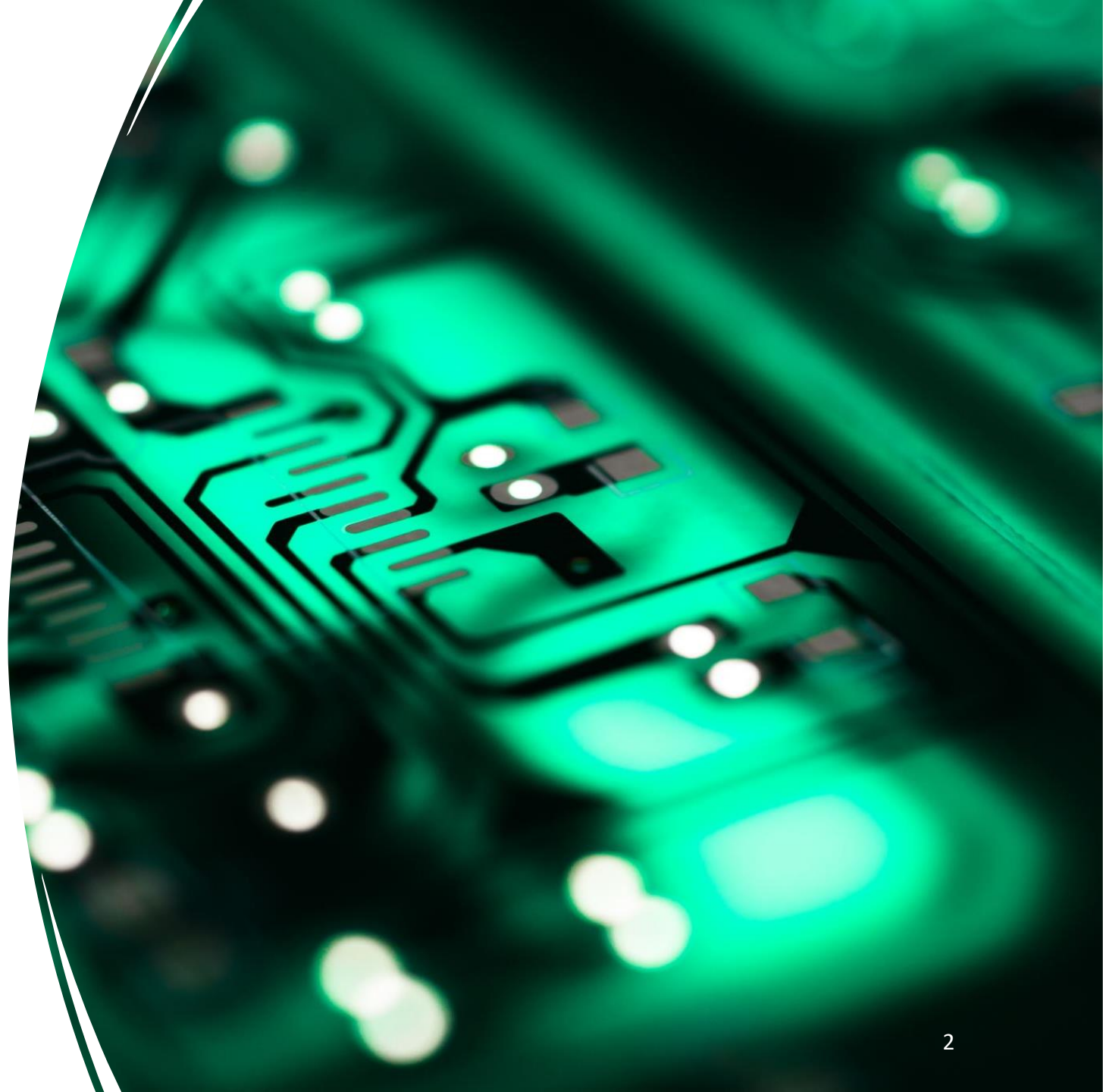
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Magnetic Materials

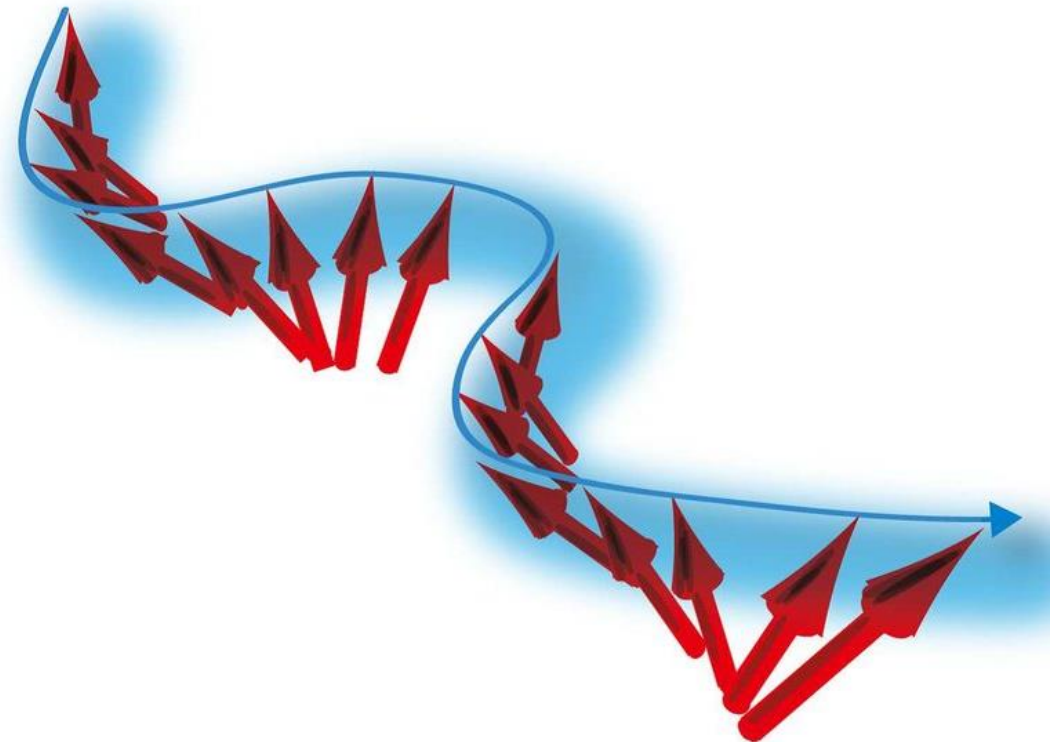
Why is understanding magnetic structures important?

- Data Storage (RAM and hard drives)
- High-resolution imaging
- Spintronics
- Superconductivity
- Quantum computing



Neutron Scattering

- Probing crystal structures and magnetic interactions by scattering neutrons off of samples
- Inelastic neutron scattering
 - Measures the difference in energy between the neutrons before and after contact with the sample
 - Creates excitations in the magnetic structure of the crystal lattice and generates a spinwave
 - Measures the energy and direction of the spinwave in a structure



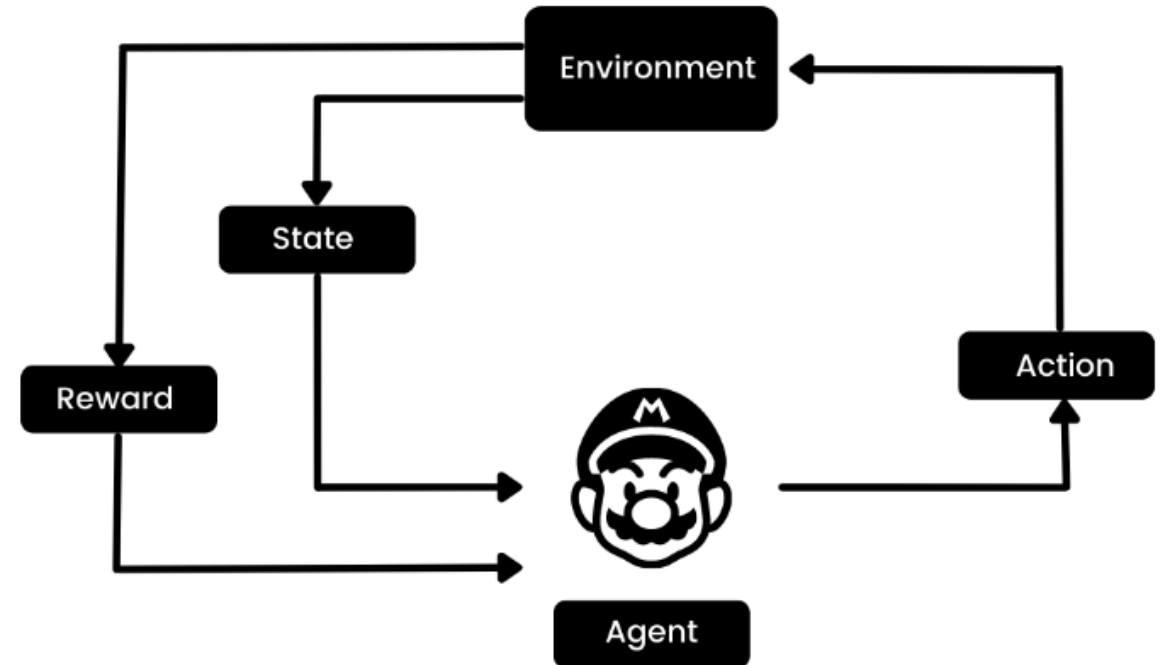
Problems

- Limited supply of neutron beams worldwide
- Experiments take a long time to run
- Not all measurements are needed

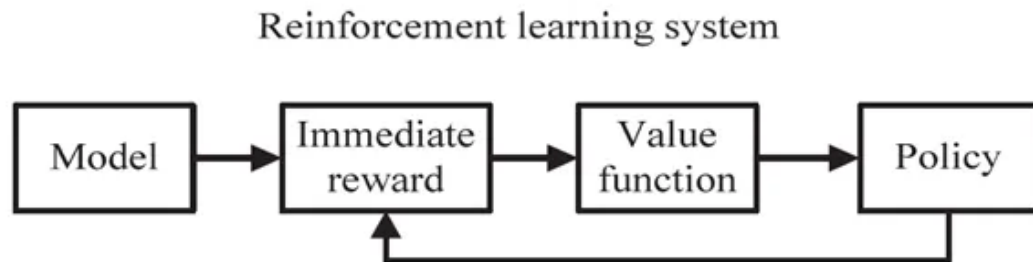


Reinforcement Learning (RL)

- Agent learns by interacting with the environment
- No data involved (unlike Active Learning)
 - Agents learn by trial and error with a reward system
 - By maximizing rewards, the agent can successfully navigate the environment

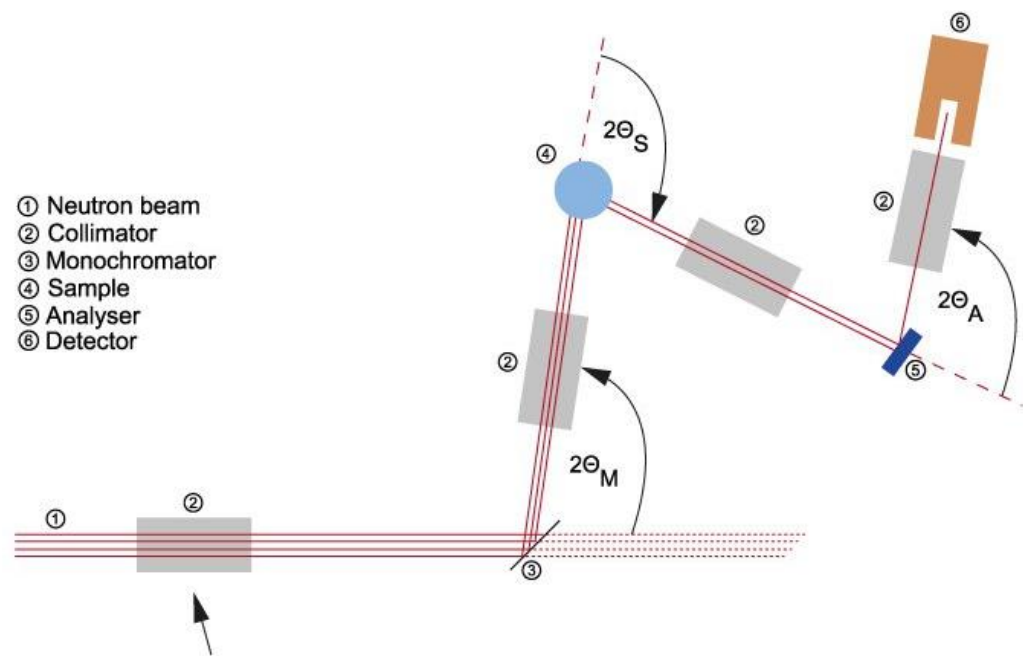


RL Process



- Observe the environment
- Decide how to act using a given strategy
- Take an action
- Receive reward/penalty
- Refine/modify strategy based on outcome
- Iterate until optimized

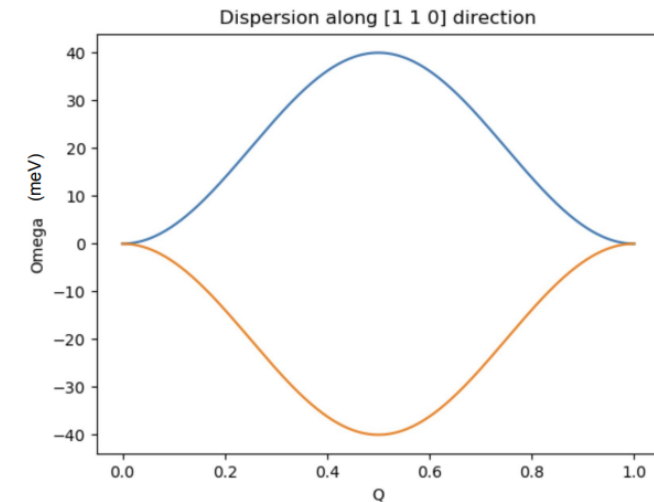
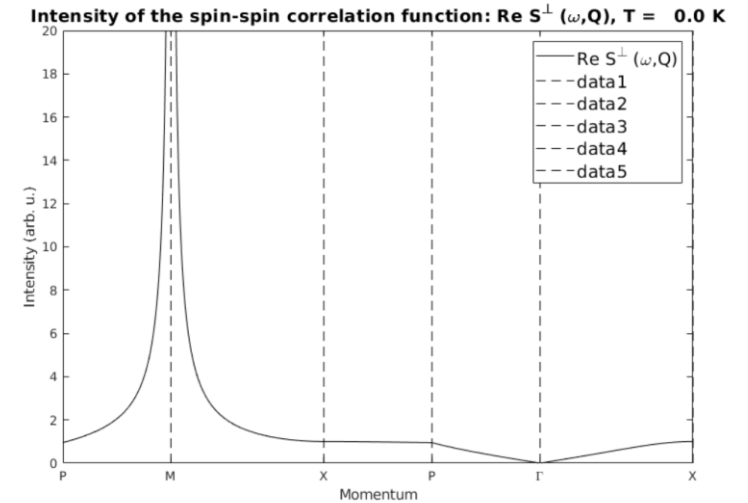
Triple-Axis Spectrometer




- First axis
 - Monochromator that filters the neutrons to a certain wavelength
- Second axis
 - Sample that neutrons scatter on
- Third Axis
 - Analyzer that selects the desired energy to be detected
- Detector
 - Detects said energy

SpinW

- MATLAB Library used to simulate magnetic structures and excitations
- Plots dispersion graphs and neutron intensities
- RL Application
 - Compiled into Python to better utilize machine learning



Challenges



- Language/Translation
- Utilizing new RL library
- Hardware limitations

Language and Translation

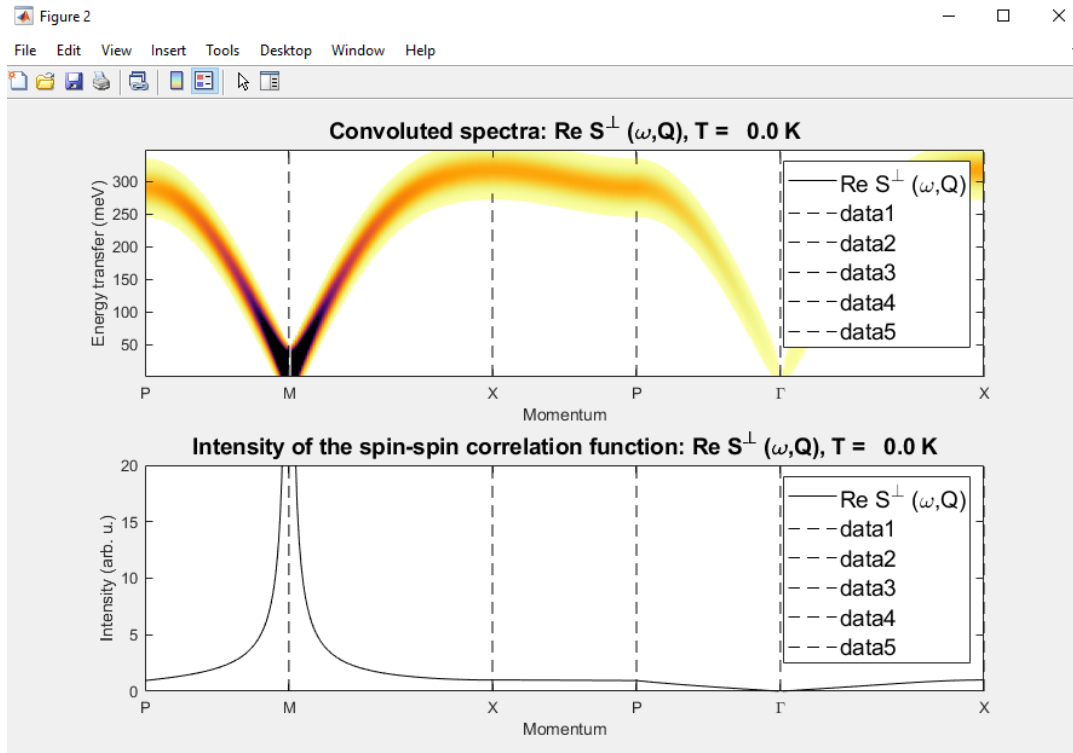
- Python-MATLAB communication
 - PySpinW (python version of SpinW) is extremely buggy
 - Cannot plot neutron intensities
- Potential Solution: Julia
 - Trouble aligning ferromagnets
 - Defined ferromagnetic structures came out antiferromagnetic

Utilized Solution:

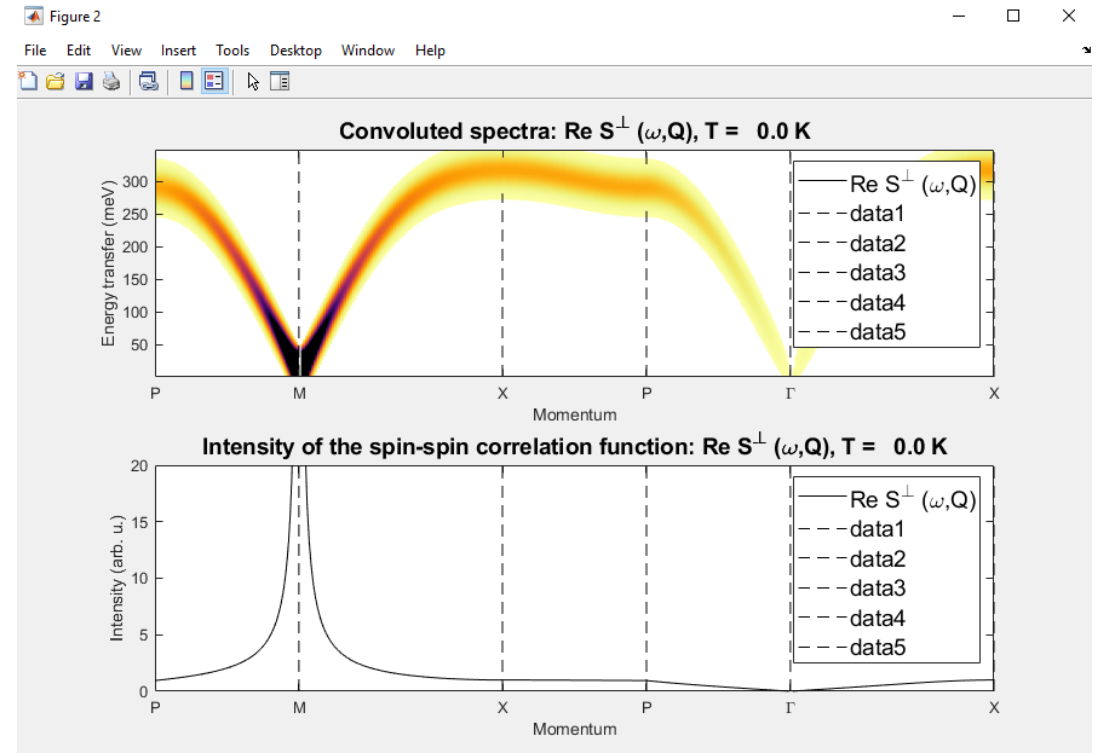
- Compile MATLAB and SpinW into python
 - Essentially calling MATLAB from Python
 - Issues with sorting arrays
 - Eigenvector sorting is scrambled when translating MATLAB to Python

MATLAB vs SpinW Neutron Intensity

MATLAB



SpinW (calling from MATLAB)



Utilizing New RL Library

- Reinforcement Learning library
 - Set of built in modules to assist with RL development
- Old RL Library is growing obsolete
 - OpenAI Gym is no longer being updated and maintained

Solution

- Switched from OpenAI Gym to Gymnasium
 - New fork of Gym library
- Reconstructed old SpinW RL algorithm to be used in Gymnasium

Hardware Limitations

- Experiments take extremely long time to run
- Memory intensive
 - Computer frequently crashes on longer experiments
 - Hard to obtain large episode datasets
- Solution
 - Parallel processing
 - Divided processing over 8 cores instead of 1
- Future Improvement:
 - Run experiments on cluster for larger datasets

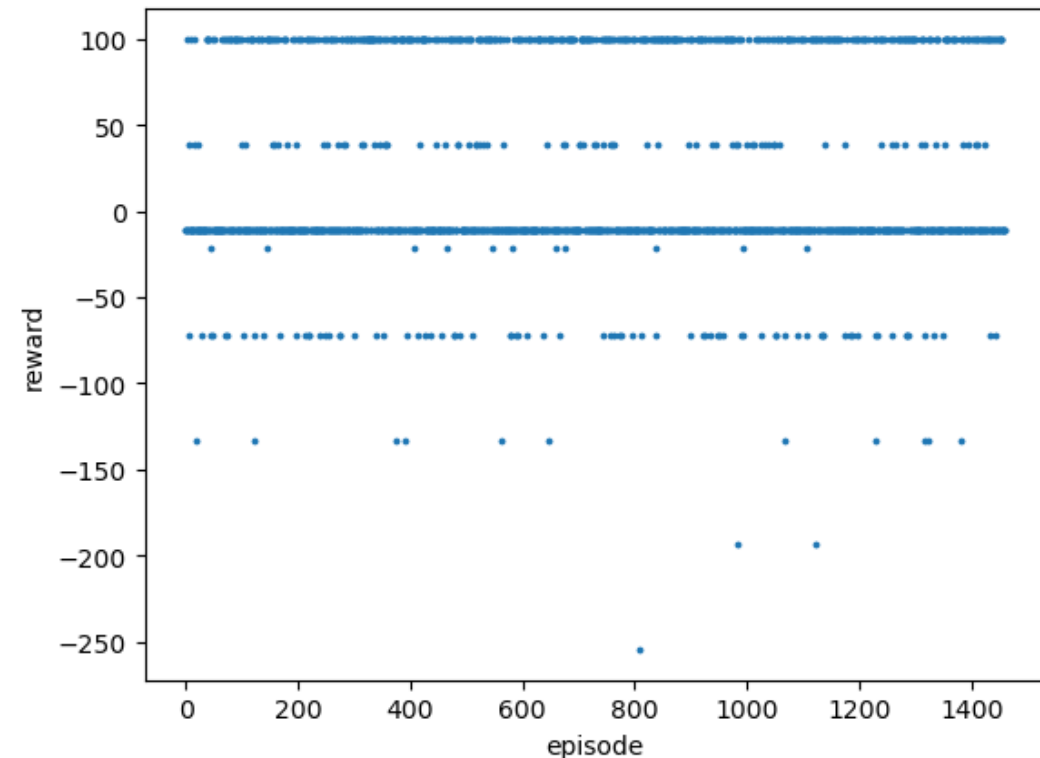
Results

- MATLAB and SpinW successfully compiled/translated into Python
 - Allows for future work to be able to plot neutron intensities in addition to spin dispersions
- RL learning process limited by hardware
 - Reward plot does not show an upward trend
 - Needs more episodes to see if it truly works



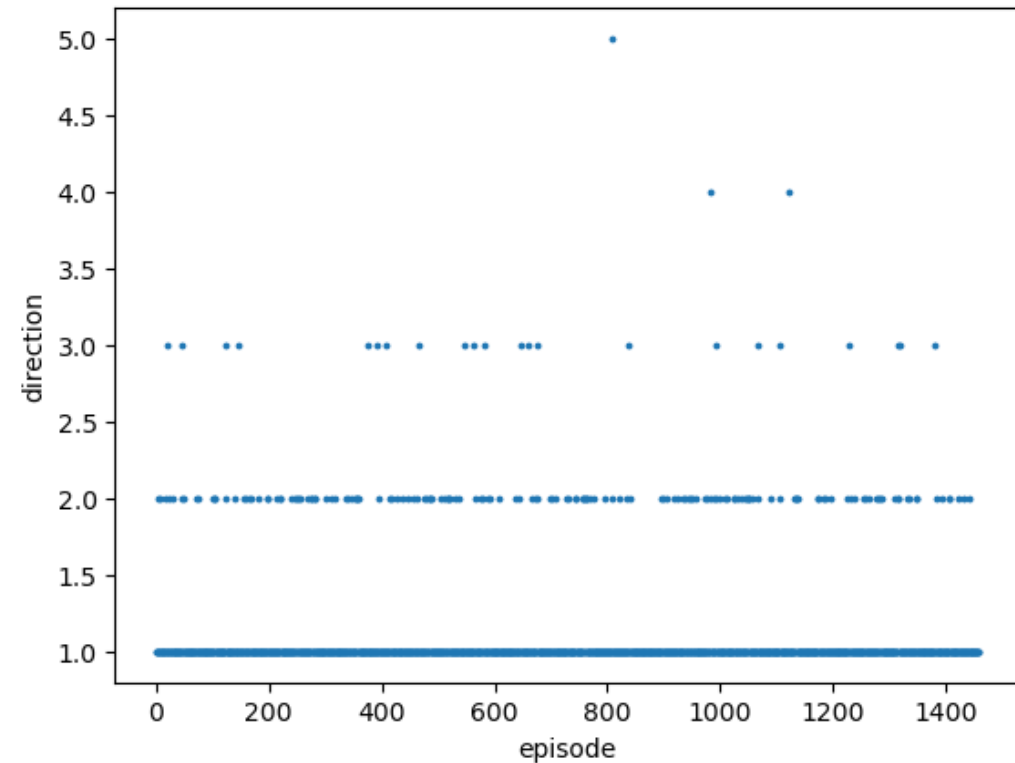
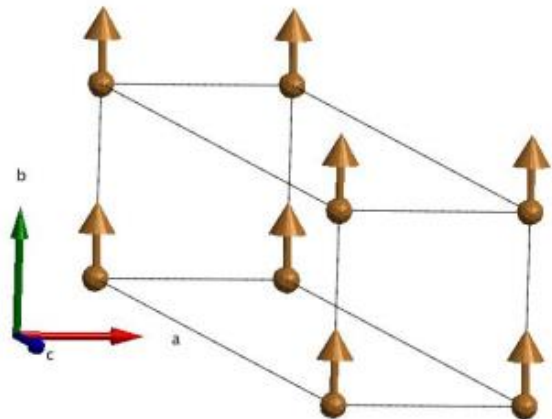
Reward/Episode

- Expectation:
 - Upward trending graph with more weight on positive rewards than negative
 - Shows that the AI is learning and slowly optimizing
- Result:
 - Relatively even all around
 - Shows that AI isn't learning very fast
 - Needs more episodes (hardware limitation)



Number of Steps/Episode

- Shows the direction to measure the spinwave dispersion
- More steps per episode means that direction is where measurements should be made



Future Steps

- Apply Neutron Intensity measurements now that it is possible
- Run on cluster to maximize episodes used and time efficiency to better train RL agent
- Publishing



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Extra Slides

Elastic vs Inelastic Neutron Scattering

Elastic

Scattered particles don't lose any kinetic energy

Can determine where atoms are from the way they scatter

Inelastic

Neutron energy changes and is monitored

Excites the nucleus

Understand energy of interactions between atoms or spins

Supervised Learning in ML

