Reinforcement Learning Algorithms for Taking Efficient Crystallographic Measurements

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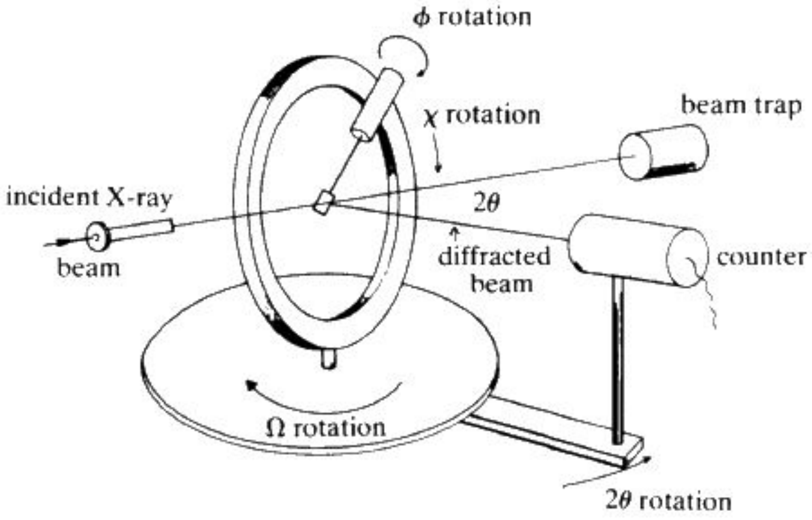
Introduction

Crystallography: Study of crystalline structures and their properties

Neutrons are a scarce resource: Neutron diffraction is time consuming and there are few facilities to perform it

Goal: Apply Artificial Intelligence to reduce beam time

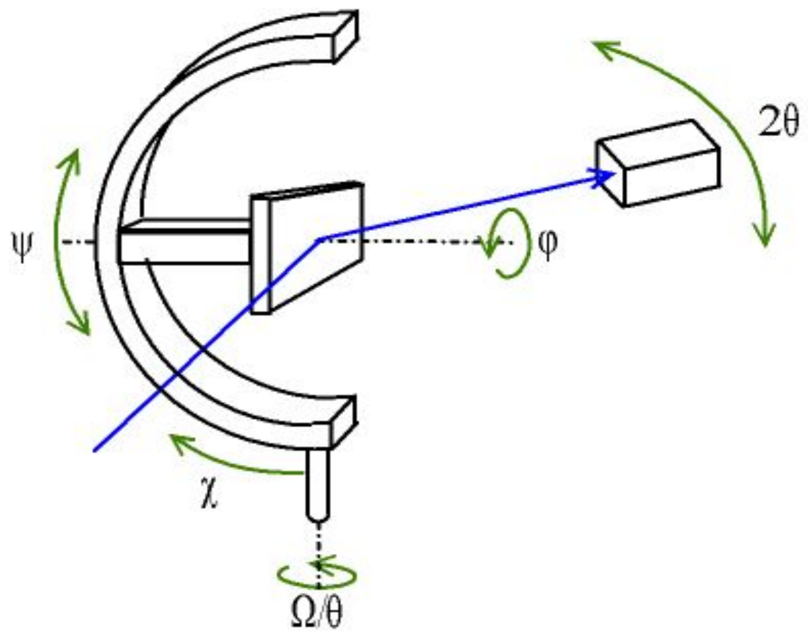


https://serc.carleton.edu/research_education/geochemsheets/techniques/SXD.html - Single Crystal Diffraction Schematic

Neutron Diffraction

- Powder Diffraction
    - Faster
    - Cheaper
    - Less Information
- **Single Crystal Diffraction**
    - **Slower**
    - **More information**

Our project is based on Single Crystal Diffraction



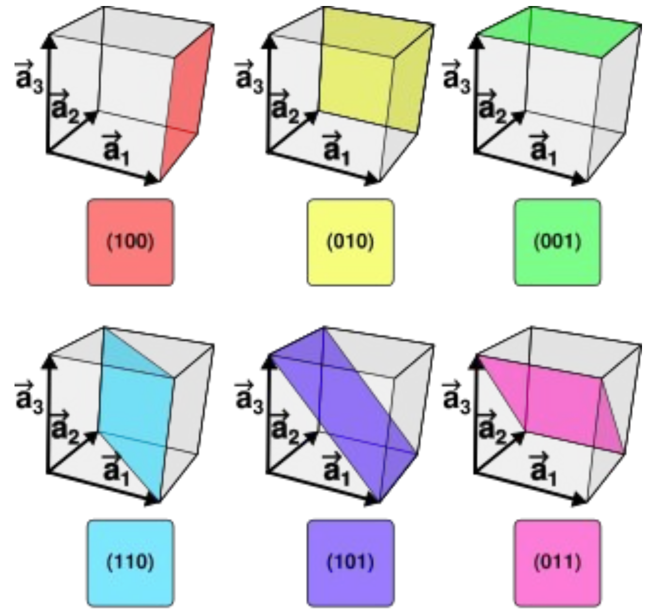
https://upload.wikimedia.org/wikipedia/commons/2/20/Diffractometre_berceau_Euler.png - Eulerian Cradle

Miller Indices (hkl’s)

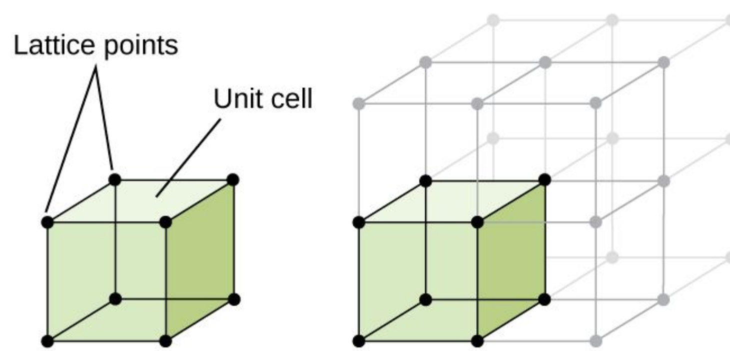
Unit cell: Smallest repeating structure; resonant of the whole structure

Miller Indices: Coordinate representations of planes in a unit cell

Instruments for rotating crystals allows us to target specific Miller indices and take measurements



https://en.wikipedia.org/wiki/Miller_index - Miller Indices



https://chem.libretexts.org - Crystal Structures

Reinforcement Learning (RL)

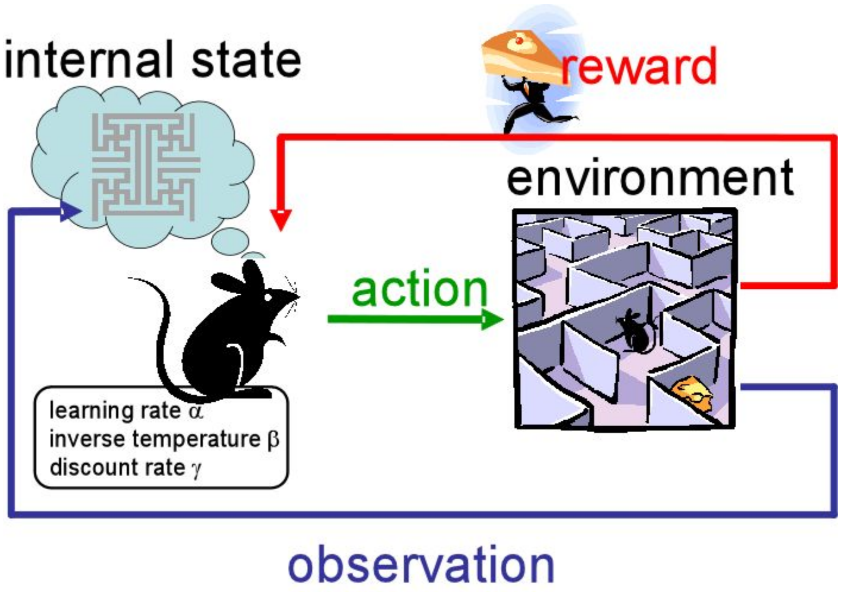
Machine Learning: Repeated Interaction with Data → “Learning”

Agent: Interacts with Environment

Environment: Returns Information

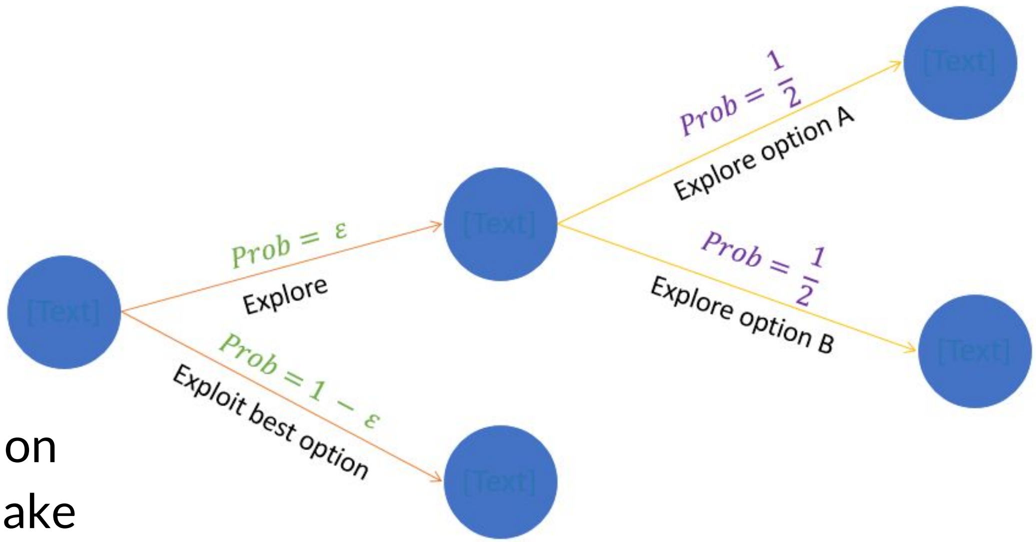
Examples: *OpenAI, Deepmind, AlphaGo, etc.*

Various Distinct Algorithms



https://becominghuman.ai/the-very-basics-of-reinforcement-learning-154f28a79071 - Becoming Human

Epsilon Greedy



Two Processes

- **Exploitation**: Capitalize on known information to make best choice
- **Exploration:** Learn more about the environment by sacrificing performance

Epsilon: Probability of exploration

https://imaddabbura.github.io/blog/data%20science/2018/03/31/epsilon-Greedy-Algorithm.html - Bandit Algorithms: epsilon-Greedy Algorithm

Methods

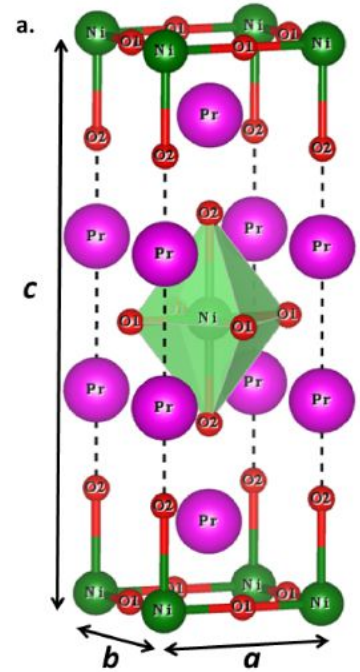
Agent: Instance of Epsilon Greedy

Environment: All Possible Miller Indices

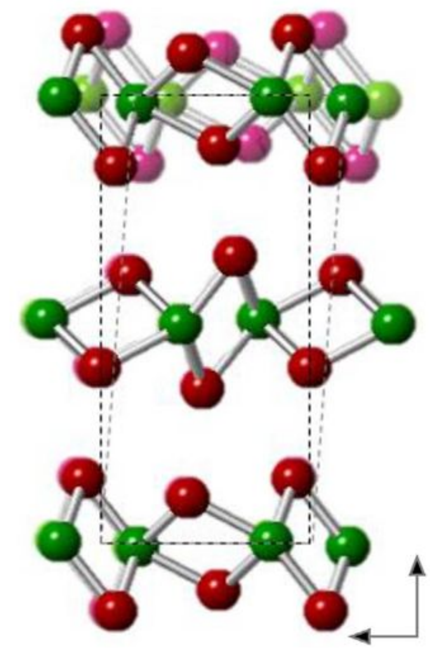
Crystals: Pr_2NiO_4, $MoTe_2$

Software and Libraries: Python, PuTTY, BLAND (pycrysfml, bumps), Docker, Linux Terminal, VR Cave

Variables: Z-coordinate approximation, starting values

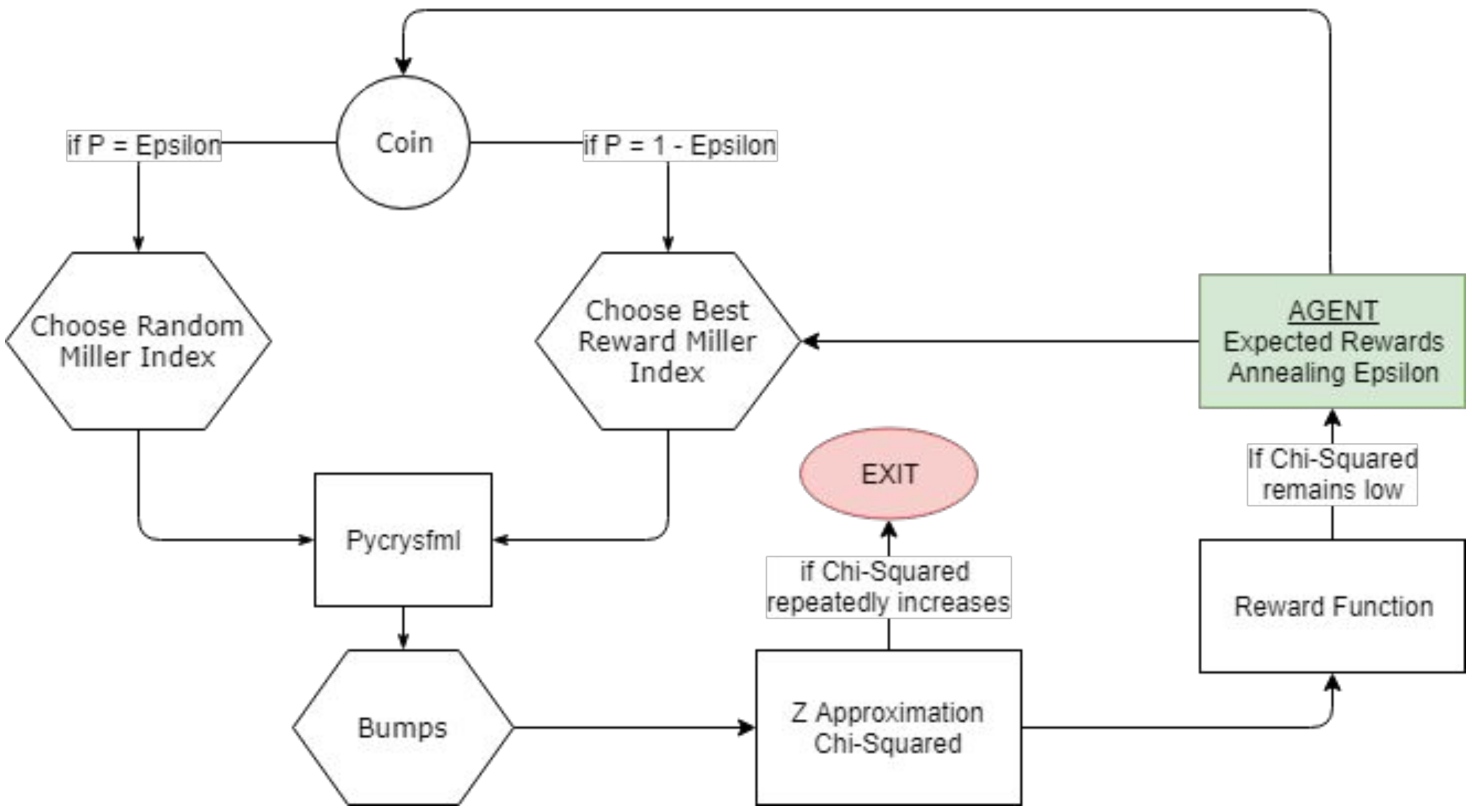


http://iopscience.iop.org/article/10.1088/0953-8984/24/40/405504 - Analysis of structural and electronic properties of Pr2NiO4 through first-principles calculations



https://www.nature.com/articles/ncomms13552 - Raman signatures of inversion symmetry breaking and structural phase transition in type-II Weyl semimetal MoTe2

Our Model



Coin
if P = Epsilon
if P = 1 - Epsilon
Choose Random Miller Index
Choose Best Reward Miller Index
AGENT
Expected Rewards
Annealing Epsilon
Pycrysfml
EXIT
If Chi-Squared remains low
if Chi-Squared repeatedly increases
Reward Function
Bumps
Z Approximation Chi-Squared

Methods

We develop and run agents using pycrysfml and bumps to efficiently select Miller Indices while finding a viable location approximation for the praseodymium or molybdenum atom.

Data Collection

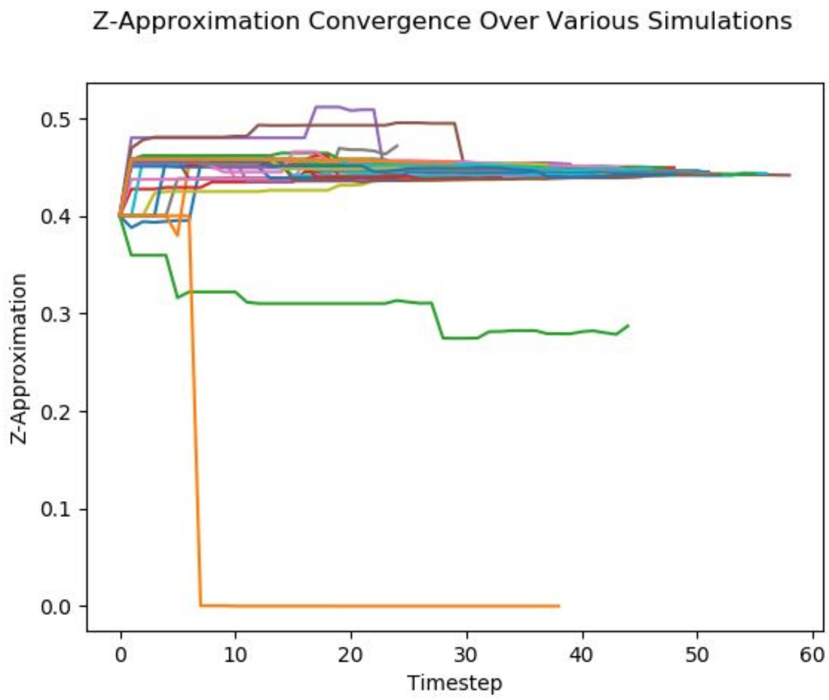
- Z-approximations for Praeseodymium/Molybdenum
- Divergence from actual Z-value (Residuals)

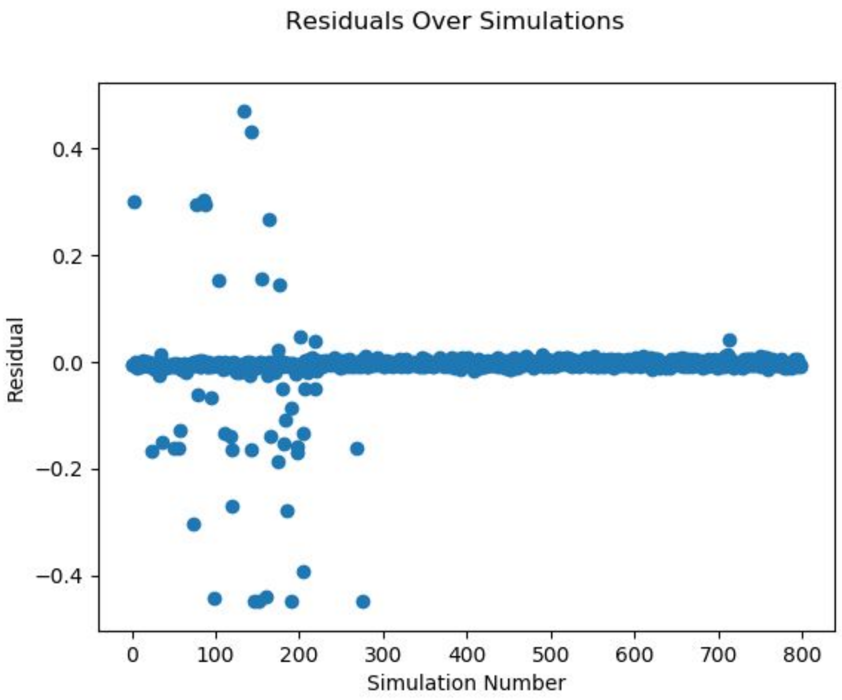
Run Specs

50 Sets x 800 simulations for each starting value and crystal

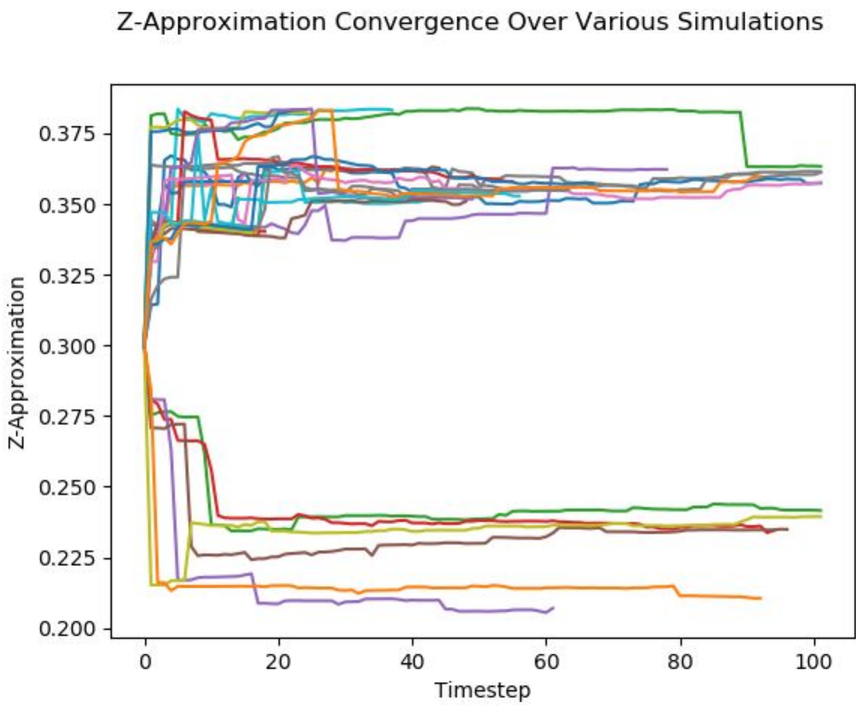
CRYSTAL	Pr_2NiO_4	$MoTe_2$
Expected Z-Approximation	Praseodymium Z Coordinate = 0.356	Molybdenum Z Coordinate = 0.449
Agent's Starting Values	{0.2, 0.3, 0.4}	{0.3, 0.4, 0.5}

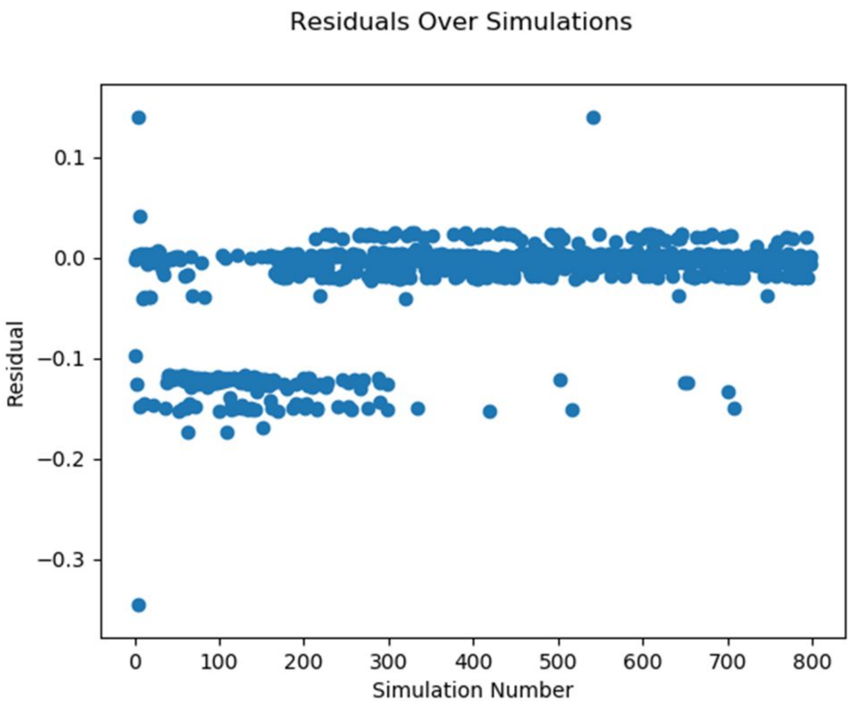
Results - $MoTe_2$





Results - Pr_2NiO_4





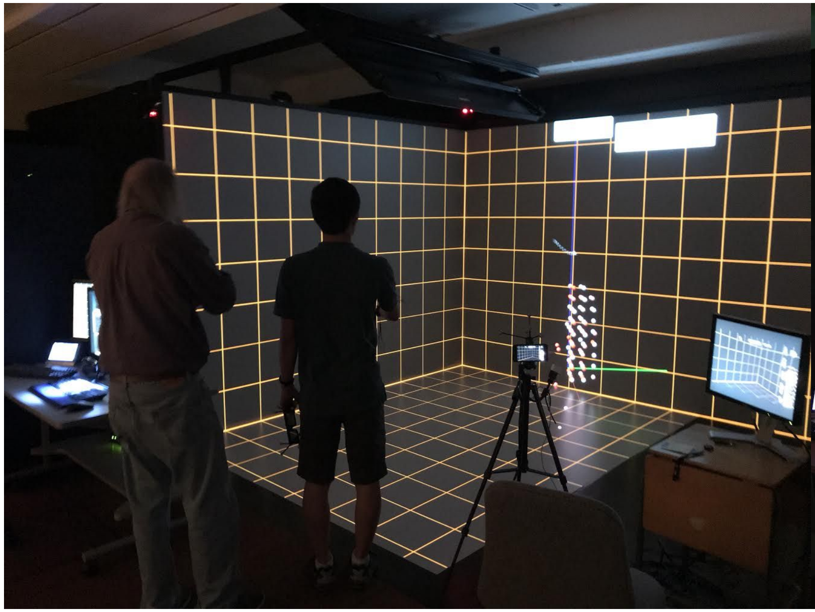
Results - Starting Points

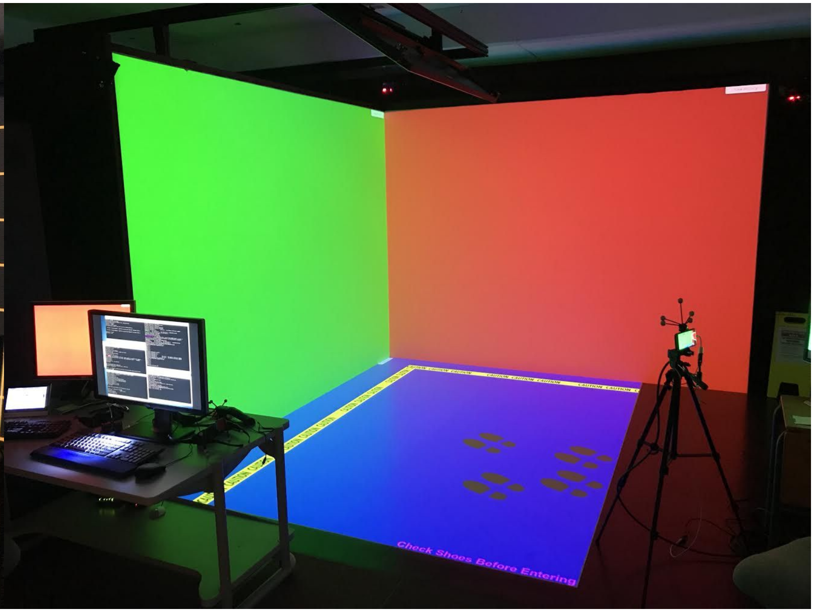
The closer the starting point was to the actual approximation, the faster and more accurately the agent converged

At some distances, there was significant improper convergence, meaning there is likely a threshold beyond which RL cannot function

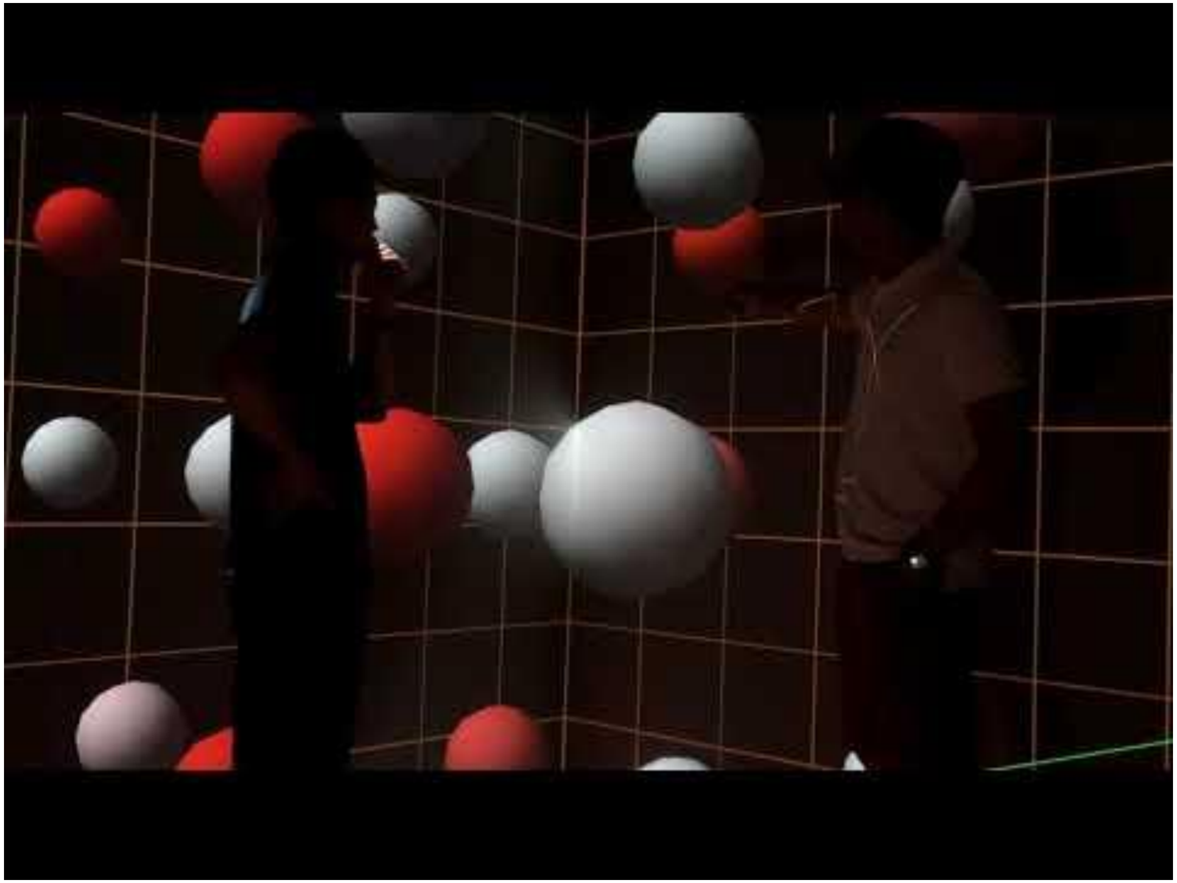
Pr_2NiO_4 (Z = 0.356)				$MoTe_2$ (Z = 0.449)			
Init. Z	0.2	0.3	0.4	Init. Z	0.3	0.4	0.5
Convergence Rate	0%	42%	60%	Convergence Rate	2%	100%	100%

Virtual Reality Cave (ITL)



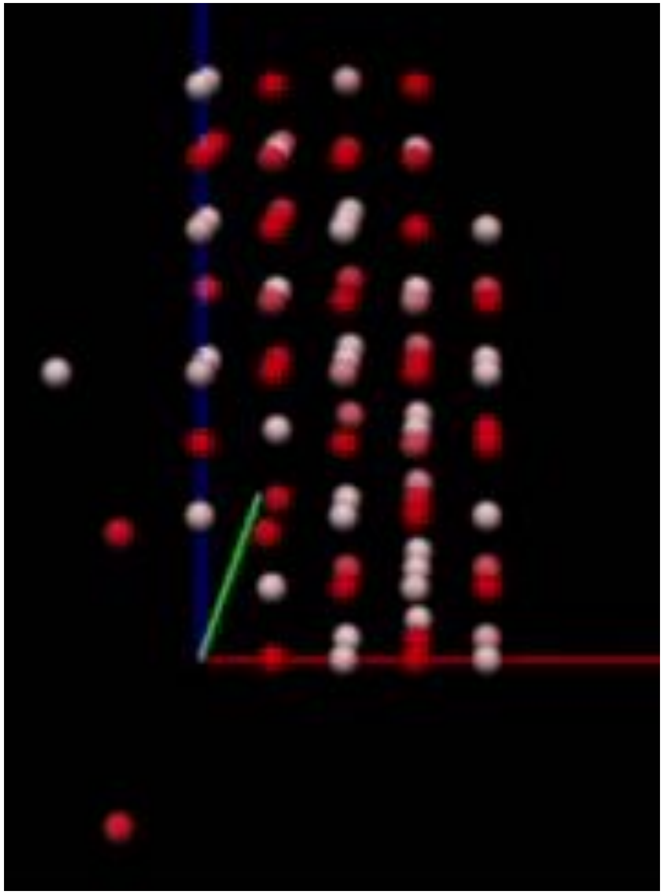


Movie Time!



Visualizing Our Algorithm

$MoTe_2$



Pr_2NiO_4

Conclusion

- Reinforcement Learning is a viable mechanism for planning efficient crystallographic measurements
- Starting parameters for RL agents are crystal-specific, and need to be adjusted per crystal
- Epsilon Greedy has limited functionality, so exploration into more advanced algorithms is warranted

Acknowledgements

Special thanks to mentors Dr. William D. Ratcliff, Steven G. Satterfield, and Judith E. Terrill.

Much thanks to Abigail Wilson, Terrence Griffin, Paul Kienzle, and Yang Zhao for their assistance

We would like to acknowledge the SHIP Program, NCNR, and ITL, as well as funding from CHRNS, and Angelique Bosse for her help with obtaining this opportunity.