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# AUTOMATION OF SAMPLE ALIGNMENT FOR NEUTRON BEAMLINES

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*Abstract*

Neutron scattering experiments are crucial for the exploration of molecular structure in compounds. The HB-2A neutron powder diffractometer at the High Flux Isotope Reactor at Oak Ridge National Laboratory conducts magnetic studies of samples by illuminating them with different energy neutron beams and recording the scattered neutrons. Proper and consistent alignment of the sample is necessary to ensure that high quality data is collected throughout an experiment. This process is currently performed manually by beamline scientists. RadiaSoft, in collaboration with the beamline scientists and engineers at ORNL, has developed a reinforcement learning-based agent capable of aligning and isolating samples. We use a Q learning structure to train the agent. The agent identifies the method to move the sample to the center of the beam and the proper amount to close the neutron camera slits. We then move the sample and close the slits using a custom Python-based EPICS IOC interfaced with the sample and slit motors. In this paper, we provide an overview of our reinforcement learning tools and show our results aligning samples like those at ORNL.

## INTRODUCTION

Automation of alignment processes for accelerators allows for increased experimentation efficiency. RadiaSoft and ORNL have been in a multi-year collaboration to develop machine learning tools for noise reduction [1], sample identification, and alignment [2]. Much of this work has focused on the TOPAZ single crystal diffractometer, but recent studies have shown success for sample alignment using the neutron camera at the HB-2A neutron powder diffractometer.

The HB-2A beamline is primarily used for magnetic structure determination [3] and services many experiments at ultra-low temperatures. It permits the application of high external fields and pressure. Its low-noise environment, paired with the constant wavelength and simple profile of its neutron beam, allows for interchangeable sample environments with minimal calibration. The beamline also permits a variety of sample changing options, allowing multiple samples to be loaded per session. A picture of the diffractometer end station is in Fig. 1.

Sample alignment at HB-2A has previously been carried out manually by beamline scientists. Automation of sample alignment would increase the efficiency of beam operations, but poses two primary challenges: the sample is not visible when not illuminated by the beam, and the presence of multiple samples necessitates slit closure to illuminate only one sample at a time. Additionally, when multiple samples are present within the beam, the beam slits must close so that only one sample is illuminated. Finding a way to overcome these challenges would streamline beam operations by reducing beam time necessary for sample alignment.

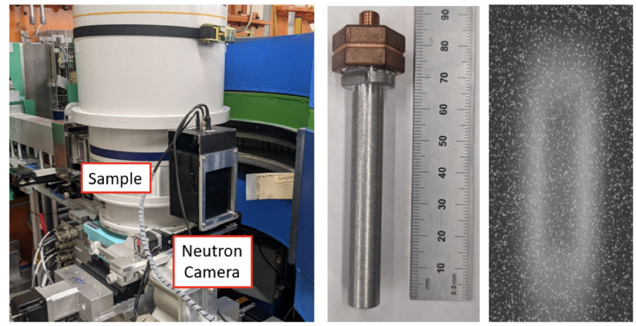


Figure 1: The HB-2A powder neutron diffraction instrument. (Left) The sample and detector area. (Middle) A standard sample holder (scale in millimeters). (Right) An example of a neutron image, with the powder sample appearing as a shadow-like image in the white beam.

## ENVIRONMENT SETUP

Our reinforcement model was trained in a custom Gymnasium environment that creates a simulated version of the HB-2A neutron camera. We simulate motor movement by moving the sample one pixel at a time in any lateral direction. An example of the simulated beamline is in Fig. 2. The reward function for the sample is defined as $-r^2$ for samples within the beam and $-r^4$ for samples outside of the beam, where r is the distance between the sample center of mass and the center of the image. When the sample is outside the beam, it is not illuminated and is therefore unable to be detected. For multiple sample images, we select one sample at a time to center and close the slits around.

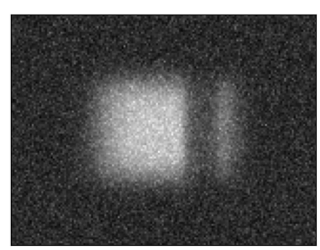

Figure 2: Neutron camera image at environment initialization.

When no sample is detected, we assign a random outside-of-beam position to the sample center. The image is rescanned every 10 steps to determine whether the sample is re-positioned within the beam. Once the sample center is located at the center of the beam (Fig. 3), the camera slits are closed so that only the sample is visible (Fig. 4).

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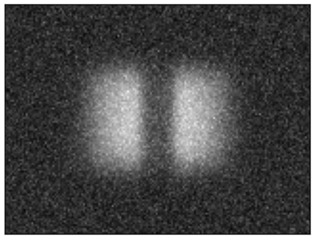

Figure 3: Camera image after sample is centered within beam.

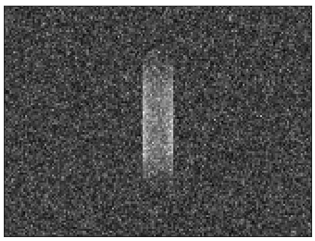

Figure 4: Camera image after slit closure.

## MODEL TRAINING

We use a U-Net model trained on data from a simulated version of the HB-2A beamline to identify the sample within the environment image, along with an epsilon-greedy policy to determine the optimal action to center the sample and train the reinforcement learning agent. The Q learning values are updated after each training episode. After training the agent on 3000 examples of the simulated beamline, we test its efficiency on both the simulated beamline and actual HB-2A images.

## MODEL RESULTS

Our RL agent was tested on 25 simulated neutron camera images with one sample within the beam and 25 total samples within multi-sample images. Samples within the testing dataset had varied sizes and weights. Testing steps follow the same structure as training steps, though we take the action with the maximum reward at each step instead of exploring the environment further. The number of steps for each testing episode was limited to 100. Figure 5 shows an example of a sample identified by the U-Net model at the beginning of its testing episode. Figure 6 shows one of multiple samples within the beam centered.

For the 25 single-sample camera images tested, agent took 47.28 steps on average to center the sample. The average number of steps necessary to center was 38.56, and the ratio of the average number of steps necessary to the average number of steps taken was 0.816.

For the multiple-sample camera images, the agent took 47.68 steps on average to center each sample and necessitated only 39.24 steps on average. The ratio of average number of steps necessary to number of steps taken was 0.823.

During training, we found that our RL agent is currently incapable of centering samples that begin outside of the neutron beam within the set number of testing steps. Our results do show a potential for a similar agent to be used for the HB-2A beamline, but further work is required to

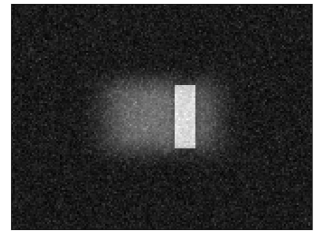

Figure 5: A sample identified at the beginning of its testing episode.

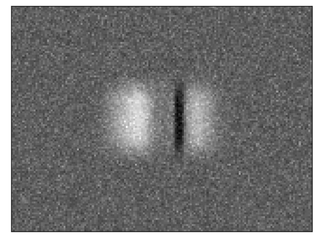

Figure 6: Two samples at the end of the testing episode for the left sample.

determine the optimal way to center a sample that begins outside of the beam.

## CONCLUSIONS

The efficiency and accuracy of our RL agent can be applied to the HB-2A diffractometer at ORNL to streamline beam operations. With the success of our agent in identifying, centering, and closing slits around samples of different shapes, sizes, and weights that begin within the neutron beam, our agent shows promising initial results. With proper adjustments to the function of the environment and agent when centering samples that begin outside of the beam, this tool could become valuable for centering samples within the HB-2A beam.

## ACKNOWLEDGMENTS

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