Run ptychography jobs on ALTAS:

* To submit a ptychography job, make sure you have the following files:
  + Ptychography software package from Yi Jiang’s fold\_slice repo on Github: <https://github.com/yijiang1/fold_slice>.
  + Job submission related files, they can be downloaded from <https://cornell.box.com/s/3vkqwdfboexuzw4fsjnvnwf3b8kq9dy7>. Put the four .m files under fold\_slice/ptycho of the ptychography software.
  + 4D Ptychography in a .mat file, with the 4D array variable name being ‘cbed’, the first two dimensions are k-space.
  + Test data for mixed state ptychography can be found on <https://www.nature.com/articles/s41467-020-16688-6>
  + Test data for multislice ptychography can be found on <https://data.paradim.org/doi/ssmm-2j11/>. The 4D array is named as ‘dp’, rename it as ‘cbed’ and save the data again.
* Then, make sure you have the following information:
  + Absolute path (start with /home/fs01) of the 4D dataset. -> second row of parameter file.
  + Absolute path of the folder to save the results. -> third row of the parameter file.
  + Experiment conditions (convergence angle, scan step size, rotation angle, etc) -> parameter file.
  + Absolute path of the parameter file. -> PARFILE of the .sub file.
  + Absolute path to the fold\_slice/ptycho folder in the ptychography software package. -> EXEPATH of the .sub file.
* For each ptychography reconstruction:
  + Open the parameter file, modify the path on the second and third row to point to the location of the raw data and the directory to save the results. Modify the rest parameter to match experimental conditions.
  + Open the submission file, modify variable EXEPATH to the location of fold\_slice/ptycho, modify variable PARFILE to point to the parameter file. Modify the requested resources accordingly, 1 GPU and 32 CPUs should be good for all the jobs.
  + Connect to ALTAS using ssh, enter the path of the .sub file, submit it with sbatch, wait for the job to finish and collect results from the result saving path.
* Benchmark tests:
  + Multislice ptychography

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| Computing resources | RTX4000 + 40 CPUs | A100 + 32 CPUs | ½ A100 + 32 CPUs | 1/3 A100 + 32 CPUs | ¼ A100 + 32 CPUs |
| Time per initialization iteration (sec) | 22.8 | 12.3 | 14.8 | 18.0 |  |
| Time per refine iteration (sec) | 74.7 | 23.7 |  |  |  |

* + Mixed state ptychography

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| Computing resources | RTX4000 + 40 CPUs | A100 + 4 CPUs | ½ A100 + 4 CPUs | 1/3 A100 + 4 CPUs | ¼ A100 + 4 CPUs |
| Time per iteration (sec) | 0.91 | 0.51 | 0.78 | 1.07 | 1.35 |