HPC workshop pt.2 (tomography datasets)

Jennifer and Matt 2/21

Agenda

- Outline
- Linux and SLURM basics; notes from items we hit during the week.
- Open OnDemand items we hit
- Overview for the datasets/challenges
- Questions for AreTomo
- Questions for Etomo

Linux basics

- How to see if the job is running?
- **How to see why a job failed?** A: view the slurm.out with `cat slurm.out` or with text editor. Errors can be challenging but may point out an issue with how the script or command was provided. Common errors include script not being able to run or a program not finding an input file correctly.
- How to edit scripts (cheat sheets for 'vi' and 'nano')
- Using ./ for local file paths vs programs in the PATH.

Useful commands

vi filename.txt	Open a new or existing file called filename.txt
vi -r filename.txt	Recover a file called filename.txt that someone was editing when the operating system crashed
view filename.txt	Display read-only filename.txt
cat filename.txt	Output contents of filename.txt; suitable for small files
less filename.txt	Output contents of filename.txt; suitable for large files; navigate using arrow keys

cat slurm<jobid>.err

cat slurm <jobid>.out

Vi cheet sheet

Saving/Exiting	:w write the file :wq write and quit :q quit :q! quit without saving
Inserting Text	i insert text before cursor a append text after cursor I insert text at beginning of line A append text at end of line
Exit a mode	<Escape Key> to exit from modes like editing or the command mode.

vi or vim are useful editors as they are standard on Linux and UNIX systems

Open OnDemand questions/notes

1. **How to copy and paste from normal desktop into the OOD desktop?**

2. **How to see why a job failed?** A: view the slurm.out with `cat slurm.out` or with text editor. How to understand the errors can be challenging, but can point out an issue with how the script or command was provided. Common errors include script not being able to run, or not finding an input file correctly.

3. **How to extend a session?** A: reach out to the HPC administrator - its possible at the admin level to extend a job or session time limit when needed.

Open OnDemand questions/notes

1. **Why doesn’t right button on 3-button mouse work in OOD session? How to recover from a frozen session?**
    1. Answer : Relaunch the OOD session; this can be done at any time and doesn't close / lose your work or windows - if something goes wrong - like a frozen window, just relaunch. This works better than refreshing the browser window.

2. **Cannot click on the 'Done' button at the bottom of the Etomo view**;
    1. Can minimize sub windows in a step. You can also move the Apple taskbar to the left side of the screen to allow a larger OOD window display. (Settings -> Display and Dock to choose left side)

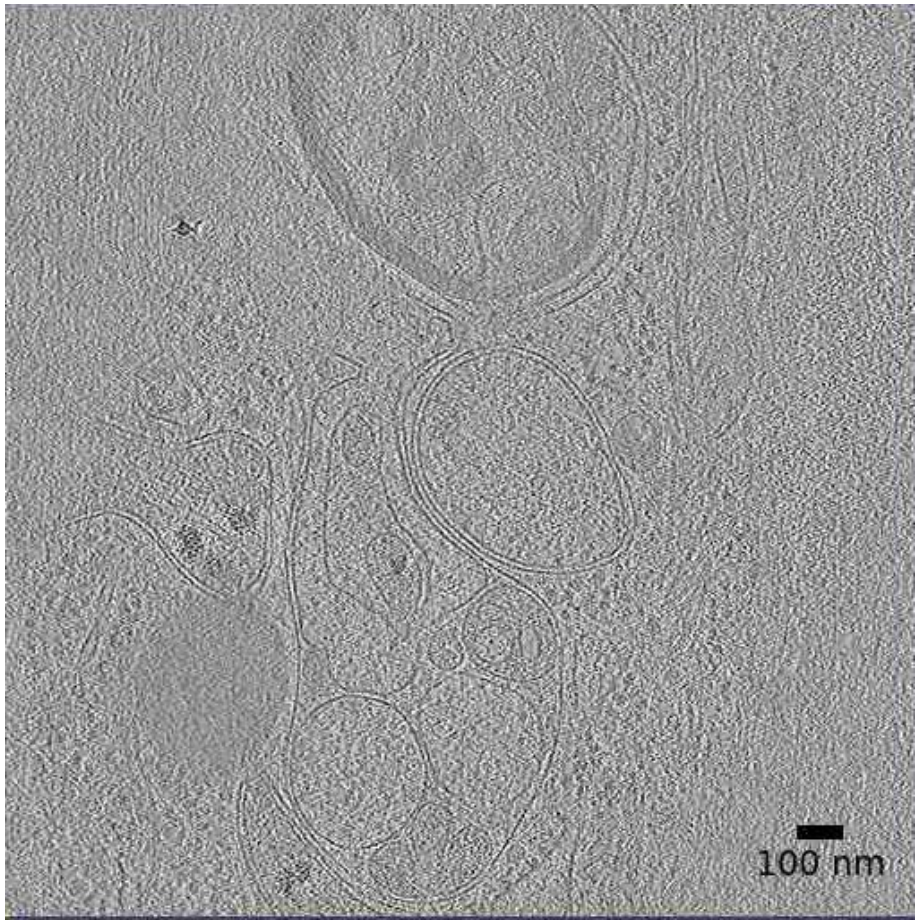
3. **What is the warning from Etomo:**

'QStandardPath: XDG_Runtime_DIR not set' (?) : appears to be about a temporary directory and may be related to how user logs in on the HPC node.

Overview for the datasets and challenges

- AreTomo example results

Cell_Lamella



$HOME/HPC_additional_sample_data/Cell_Lamella/output2/tomogram.mrc

Tried smaller –AlignZ 800
Tried larger –VolZ 2000

Seemed to catch entire contents, and a little better detail than example.

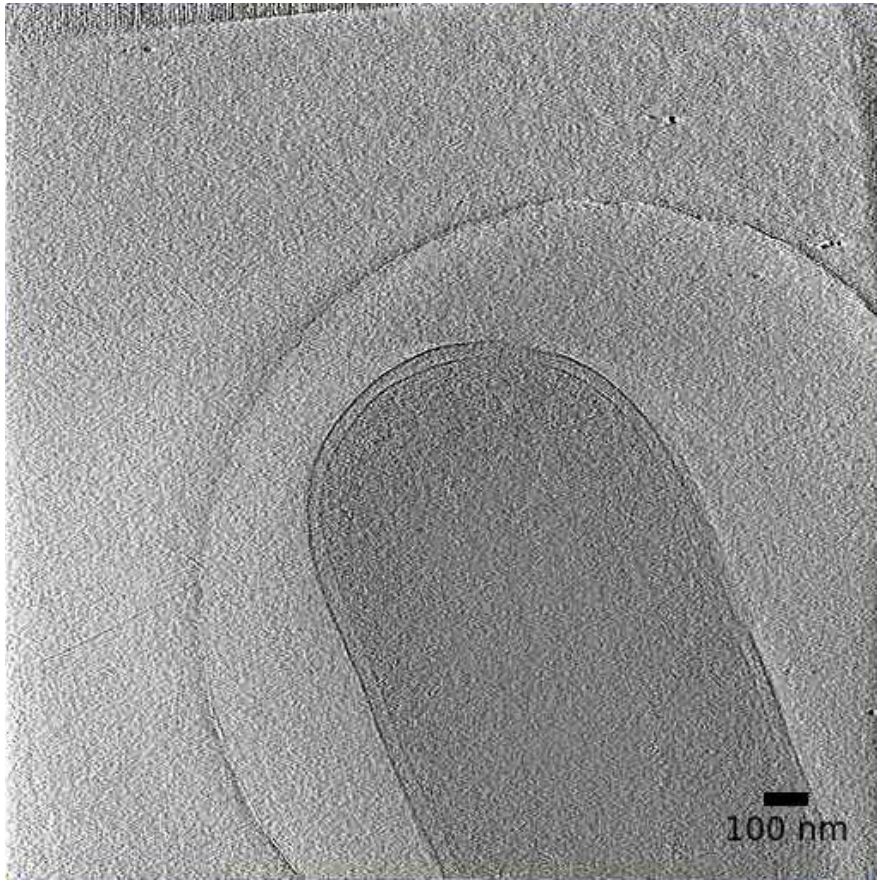
(No IMOD comparison)

~~- IMOD example results~~

Overview for the datasets and challenges

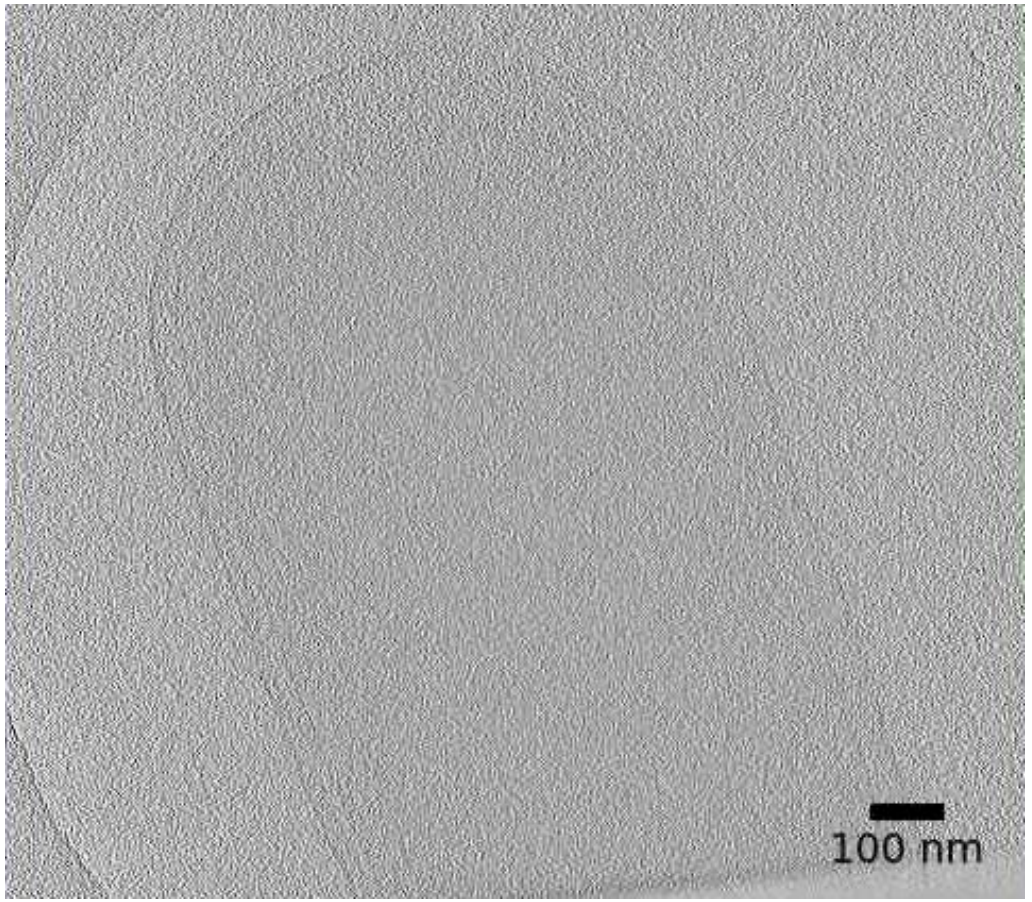
- AreTomo example results (try 3)

Bacteria (VolZ 3200, AlignZ 800);
initially very bad – separation as you tilt



- IMOD example results

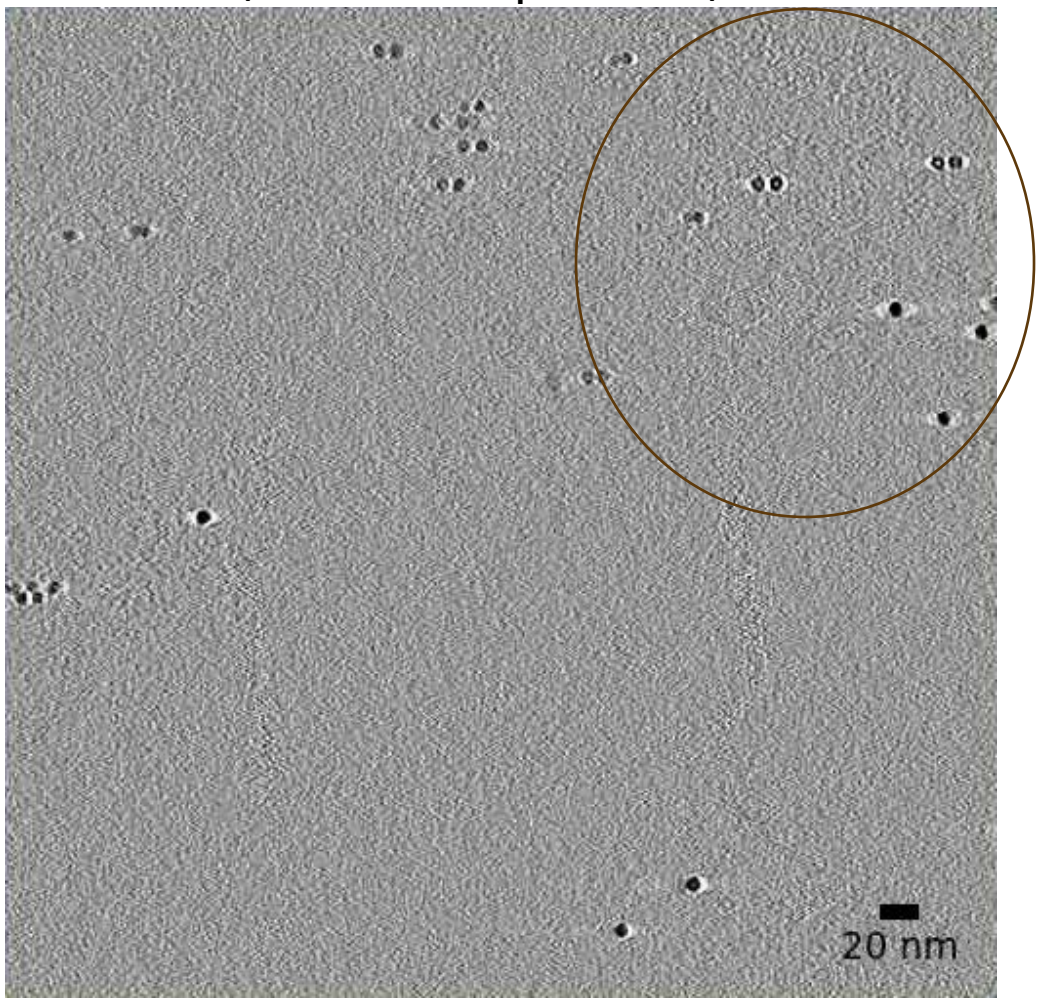
Could get more crisp membranes, contrast is a bit difficult; bin6 shown below



Overview for the datasets and challenges

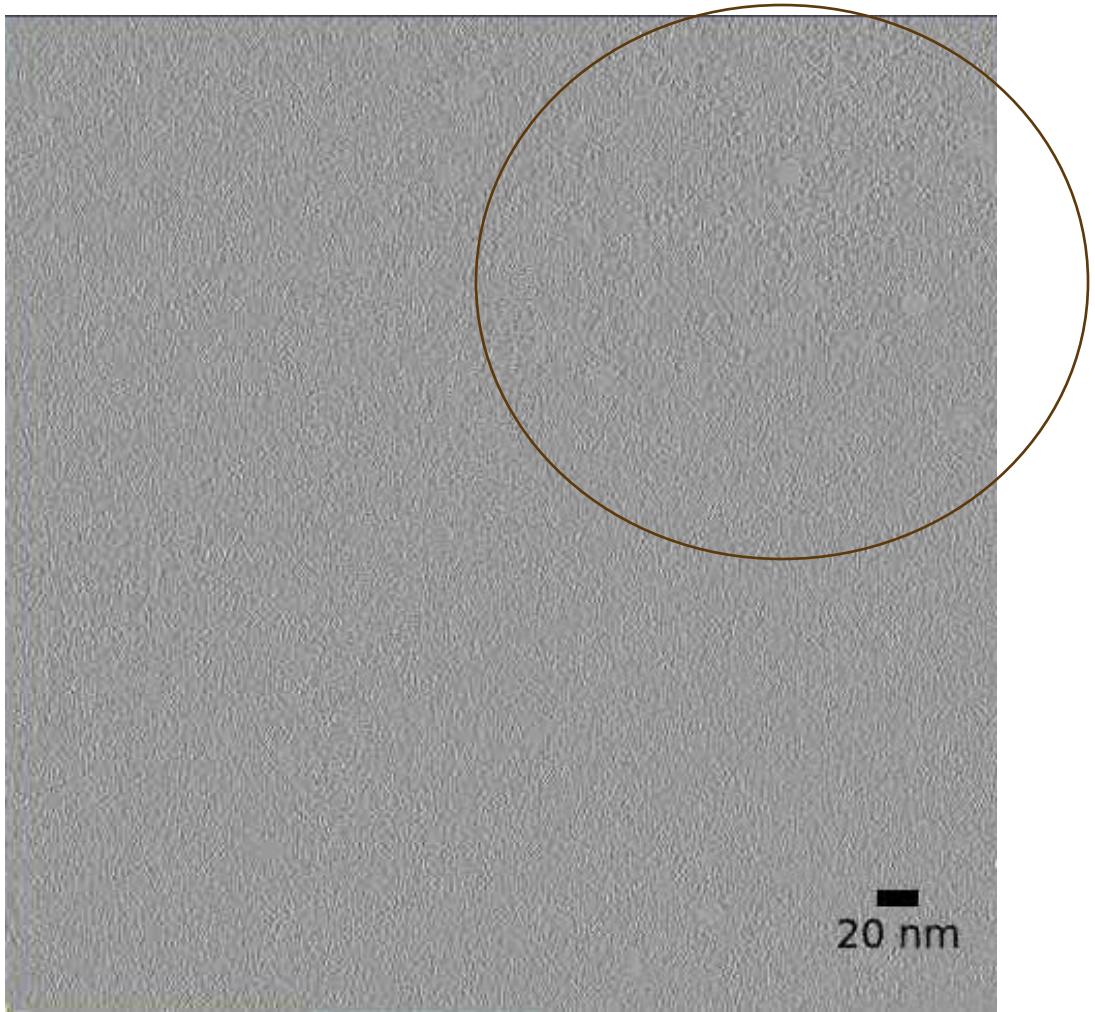
- AreTomo example results

  DPS (hard to see particles)



- IMOD example results

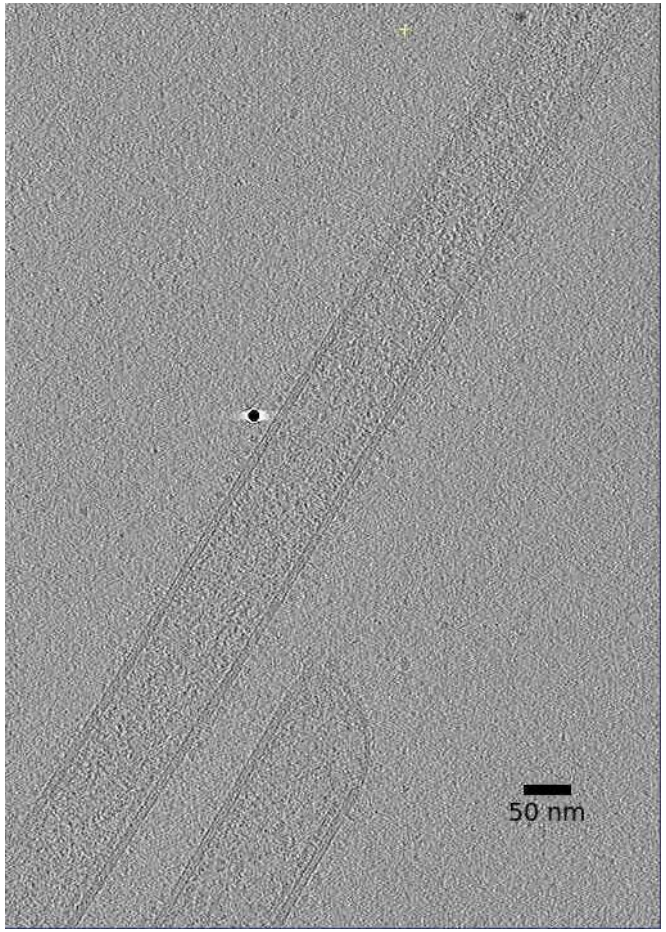
  Fiducials erased, alignment by fiducials can see more DPS on more Z slices.



Overview for the datasets and challenges

- AreTomo example results

  RSV (w17_g1_ts_013_ali)



- IMOD example results

  Could reach alignment error (0.1588, 0.107nm sd), and leave-out error of 0.2395 nm.

AreTomo questions

1. What parameters are most important to focus on?

2. What were the most challenging datasets?

Etomo questions

1. (Matt) w17_g1_ts_013_ali, in the Preprocessing - I can see peaks during the find X-rays step, but the corrected stack doesn't change the min/max values. Should we adjust the peak criterion to remove outliers and how? How critical is the preprocessing and is this always used?

2. How to tell when you are at a good stopping point in `Fine Alignment` and adjusting the fiducial positioning?

3. How to better see boundaries in the Image XYZ view during Tomogram Positioning? Sometimes very faint boundary between the edge of the ice and space.

4. Do you always run CTF Fitting steps in Etomo for a tomogram? Some datasets clearly showed peaks that could be fit, while others did not? (Examples). Are there good strategies here for the CTF Fitting?

5. Do you always want to erase gold beads? Will this also improve quality for the final tomogram? If this step doesn't find all the beads such as those at only farther tilts, how can you improve? (Examples)
6. How to get improved contrast from the tomograms?

Wrap up!

- Was this useful and would you like to do similar workshops in the future?
- Survey link: https://uwmadison.co1.qualtrics.com/jfe/form/SV_8cysE5RfiI4iOeq

Thanks!