

Remote Applications Training Agenda

CryoSPARC data processing

University of Nebraska-Lincoln, Jan 15-16, 2025

Disclaimer: The following agenda is suggested and subject to change. Application personnel will try to be flexible based on customer experience and requests.

Format: remote training

Instructor: Helen Donelick

Day 1: (Jan 15th) CryoSPARC processing with example dataset

Start: 10am (CST)

Lunch: 1pm

End: 5pm

Before remote session

- Ensure all attendees have access to local computational resources.
 - o Example dataset (commonly Apoferritin or a proteasome) is on local resource and the attendees can access the dataset
 - o Attendees have CryoSPARC login credentials

Brief presentation:

- Basics of data processing and our goals

Go through workflow of CryoSPARC.

- Import movies.
 - o Discussion of required parameters
- Motion correction and CTF estimation.
- Blob picking and template picking.
 - o Why we start with blob picking.
 - o Deciding on templates to use.
 - o Inspection of picks manually.
- Particle extraction and 2D classification.
 - o How to decide box sizes.
 - o good vs bad 2D classes.
- Ab-initio reconstruction.
 - o Why we use this feature.
 - o what are we looking for.
- Refinement.
 - o How can we push the resolution without overfitting.
 - o Differences between homogenous and heterogenous refinements.

Examine results in Chimera.

- Explore results of ab-initio and refinements.
- Fitting models into maps.

Answer remaining questions.

Learning Objectives:

- By the end of the day, the participants will be able to:
 - o Access their local computational resources.
 - o Understand the basic workflow of CryoSPARC.

- Evaluate results in Chimera.

Day: (Dec 16th) CryoSPARC processing with example dataset- Group 2

Start: 10am (CST)

Lunch: 1pm

End: 5pm

Before remote session

- Ensure all attendees have access to local computational resources.
 - Example dataset (commonly Apoferritin or a proteasome) is on local resource and the attendees can access the dataset
 - Attendees have CryoSPARC login credentials

Brief presentation:

- Basics of data processing and our goals

Go through workflow of CryoSPARC.

- Import movies.
 - Discussion of required parameters
- Motion correction and CTF estimation.
- Blob picking and template picking.
 - Why we start with blob picking.
 - Deciding on templates to use.
 - Inspection of picks manually.
- Particle extraction and 2D classification.
 - How to decide box sizes.
 - good vs bad 2D classes.
- Ab-initio reconstruction.
 - Why we use this feature.
 - what are we looking for.
- Refinement.
 - How can we push the resolution without overfitting.
 - Differences between homogenous and heterogenous refinements.

Examine results in Chimera.

- Explore results of ab-initio and refinements.
- Fitting models into maps.

Answer remaining questions.

If time remains, discuss other commonly used CryoSPARC jobs.

Learning Objectives:

- By the end of the day, the participants will be able to:
 - Access their local computational resources.
 - Understand the basic workflow of CryoSPARC.
 - Evaluate results in Chimera.

Applications support summary.

Estimate of days used for this session: 2 (16 remote hours)