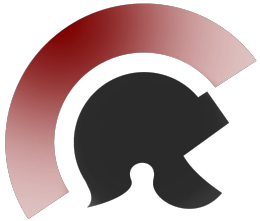
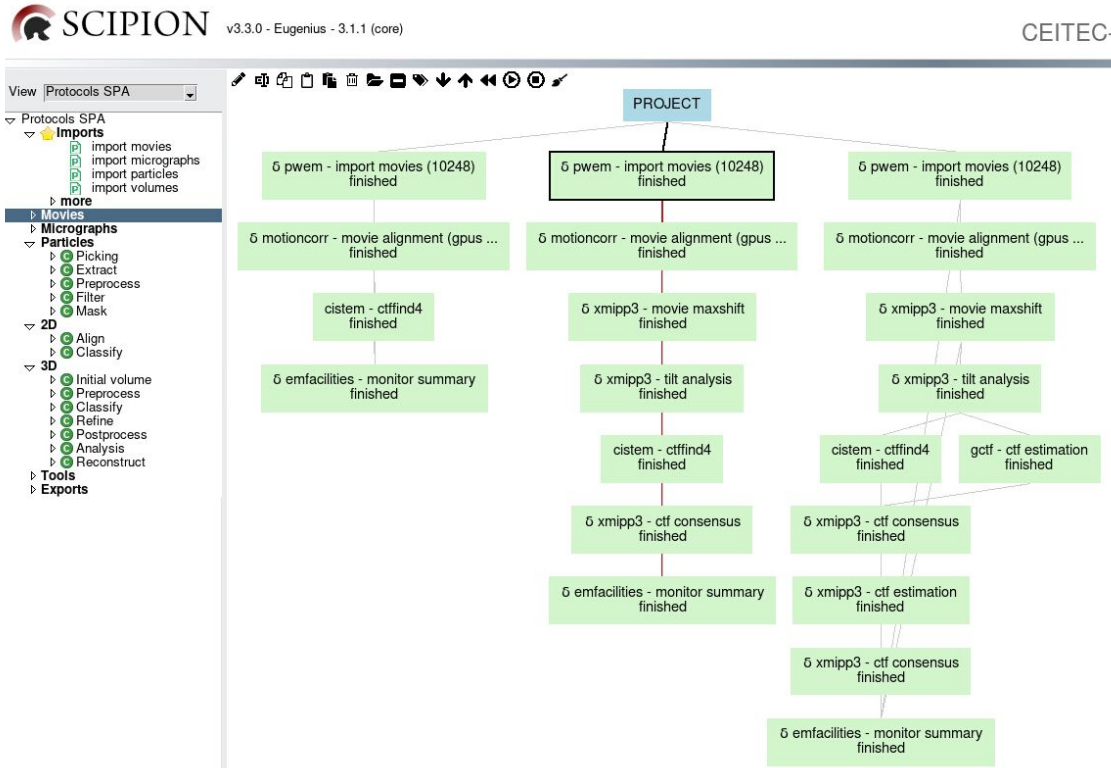


Scipion CEITEC

Cryo-EM facility workflows - The easy way

Index

1. Objective.



Create a set of generic and automatic workflows that are able to:

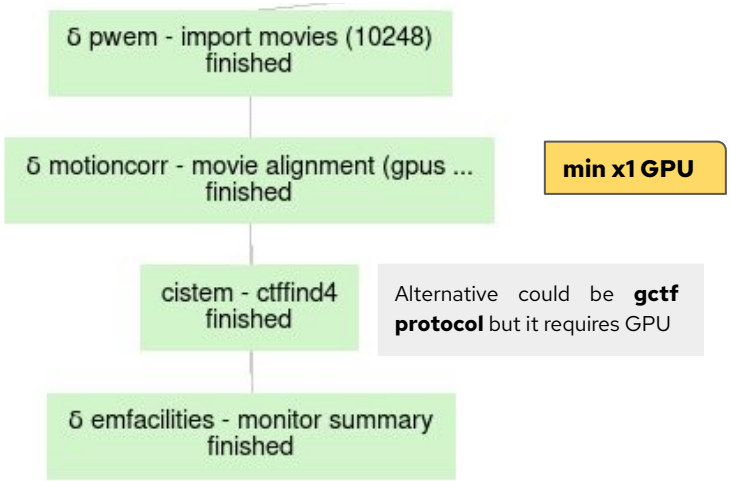
- Run on-the-fly and unattended
- Are robust and stable for a great variety of samples
- Goes from **movies** to **CTF estimation** (for the moment)
- We have **three proposed workflows**, each of them with one layer of complexity added.

*These workflows are **highly configurable**, and the facility can add and design its own image analysis pipeline based on their needs.

2. Workflows. Layer 0

Layer 0

- **Basic processing pipeline**
  - Import movies
  - Movie alignment (recommended 2 GPUs)
  - CTF estimation
- **Monitor acquisition**
  - Monitor summary:
    - Monitor basic parameters (item counts, drift, resolution, astigmatism, defocus, etc.)
    - Raise alarms (mail setting available)
    - Provides information of the basic steps (html report)
- **Feedback to the user**
  - Monitor summary: html report
- **Challenges:**
  - Is all our data and estimations really useful?



- Simple to use (4 protocols).
- Able to monitor acquisition.
- Base steps for further processing.
- Feedback to the users.
- Stream processing.

2. Workflow. Layer 1

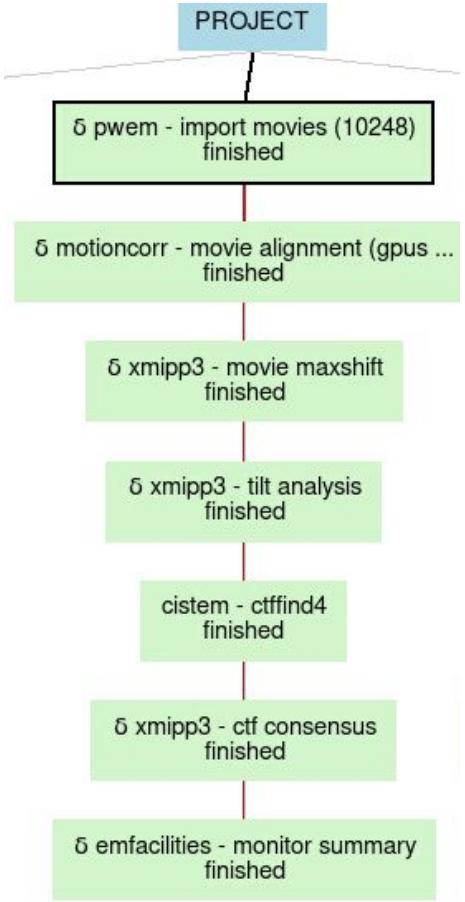
Layer 1

Improve the **quality** of the **acquisition images**:

- **Quality control protocols**
  - Movie max shift: automatic reject those movies whose frames move more than a given threshold.
  - Tilt analysis: quality score based in the Power Spectrum Density (astigmatism and tilt)
  - CTF consensus: acts as a filter discarding micrographs based on their CTF (limit resolution, defocus, astigmatism, etc.).

- **Advantages:**
  - More control of the acquisition quality
  - Reduce unnecessary processing time and storage

- **Challenges:**
  - How reliable are our estimations?

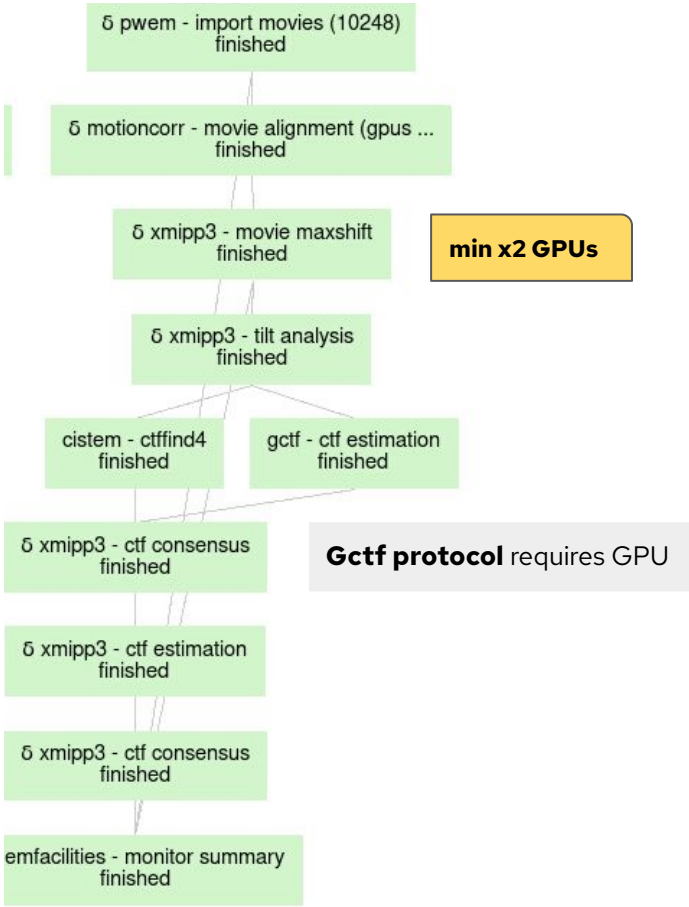


2. Workflow. Layer 2

Layer 2

Improve the **quality** of both the **acquisition** and **processing data**:

- **Quality control protocols**
  - ...
- **Combination of methods**
  - CTF consensus
    - New methods to compare ctf estimations
    - CTF xmipp criteria (richer parameters i.e. ice detection)
- **Advantages:**
  - More control of the acquisition quality
  - Robust estimations to continue with the processing
- **Challenges:**
  - Requires one extra gpu (gctf)
  - Gctf only available for CUDA 10.1



3. Implementation. Softwares

These workflows proposal is complex and requires from several external softwares (5 plugins) that are incorporated in form of Scipion plugins (scipion-em-plugin):

Scipion plugins

a. Cistem (ctf estimation)
b. Emfacilities (monitor summary)
c. Gctf (ctf estimation)
d. Motioncor2 (movie alignment)
e. Xmipp (several protocols)

Additional information:

- Motioncor2 requires GPU
- Gctf only works with CUDA 10.1
- Gctf requires GPU

4. Questions.

- The templates of these workflows should be dynamic or static templates?

- Where to store this templates?
  - Workflows will be uploaded by the Scipion CNB team in WorkflowHub

- Where to hang the monitor summary protocol in layers 1 and 2?
  - You want to see all the images or just the ones that pass our filters?

- Any request to change any of the workflows?