



How to Modify Cryosparc Script

Cryosparc Log Analysis

① Copy the path to investigate the log of the failed task.

The screenshot displays the CryoSPARC web interface. At the top, the breadcrumb navigation shows: CryoSPARC > P1 BMT-10G-h100 > W1 Data Processing > J5 Patch Motion Correction. The main area is divided into three sections:

- Event Log:** Shows a list of tasks. The selected task (J5) has a log entry for processing 1104 of 2753 movies. The log text includes:

```
[CPU: 1.87 GB] -- 1.0: processing 1104 of 2753: J1/imported/014806993408881431767_CB1_01110_Feb19_20.14.03.tif
loading /proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J1/imported/014806993408881431767_CB1_01110_Feb19_20.14.03.tif
Loading raw movie data from J1/imported/014806993408881431767_CB1_01110_Feb19_20.14.03.tif ...
Done in 1.17s
Loading gain data from J1/imported/CountRef_CB1_00826_Feb19_14.19.25.mrc ...
Done in 0.00s
Processing ...
Done in 3.72s
Completed rigid and patch motion with (Z:6,Y:5,X:6) knots
Writing non-dose-weighted result to J5/motioncorrected/014806993408881431767_CB1_01110_Feb19_20.14.03_patch_aligned.mrc ...
Done in 0.04s
Writing 120x120 micrograph thumbnail to J5/thumbnails/014806993408881431767_CB1_01110_Feb19_20.14.03_thumb_@1x.png ...
Done in 0.00s
Writing 240x240 micrograph thumbnail to J5/thumbnails/014806993408881431767_CB1_01110_Feb19_20.14.03_thumb_@2x.png ...
Done in 0.00s
Writing dose-weighted result to J5/motioncorrected/014806993408881431767_CB1_01110_Feb19_20.14.03_patch_aligned_doseweighted.mrc ...
Done in 0.04s
Writing background estimate to J5/motioncorrected/014806993408881431767_CB1_01110_Feb19_20.14.03_background.mrc ...
Done in 0.00s
Writing motion estimates...
Done in 0.00s
```
- Micrographs:** A grid of 1,120 micrographs is shown, with a red box highlighting a specific area. Below it, a section for 'Micrographs incomplete' shows 1,633 exposures.
- Details Panel:** Provides metadata for the task 'Patch Motion Correction'. It shows the title 'New Job J5', workspace 'W1', and status 'Failed'. The 'Directory' field contains the path: `/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5`. A red arrow points to this field with the text 'click'.

Cryosparc Log Analysis

② View the job log.

➤ `$ cat /proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5/job.log | grep oom`

```
slurmstepd: error: Detected 1 oom-kill event(s) in StepId=xxxxxxxx.batch. Some of your processes may have been killed by the cgroup out-of-memory handler.
```

If an OOM log is detected, increase the number of cores and rerun the task.

Creating Cryosparc Batch Script

③ Clear the processed data.

The screenshot shows the 'Patch Motion Correction' job details. The 'ACTIONS' menu is expanded, and the 'Clear Job' option is highlighted with a red box. Other options include Queue Job, Kill Job, Restart Job, Mark Job as Complete, Link Job, Move Job, Clone Job, Clear Intermediate Results, Export Job, Unlink Job from Workspace, Delete Job, Create Blueprint, and Create Workflow.

2. Clear job

1. Actions

④ Rebuild the task and immediately stop it by clicking the killed button after submitting.

The screenshot shows the 'Patch Motion Correction' job details. The 'Queue' button is highlighted with a red box. Below the job details, the 'ACTIONS' menu is expanded, and the 'View Job' button is highlighted with a red box.

3. Queue

4. Actions

Description.

This is a task to leave only the script file..

5. kill job

The screenshot shows the 'Patch Motion Correction' job details. The 'ACTIONS' menu is expanded, and the 'Kill Job' option is highlighted with a red box. Other options include Queue Job.

Cryosparc batch script 수정

⑤ Access the terminal and navigate to the folder of the task (refer to ①).

- \$ cd /proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5
- \$ pwd
- \$ ls

```
[bmttest@olaf1 J5]$ cd /proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5
[bmttest@olaf1 J5]$ pwd
/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5
[bmttest@olaf1 J5]$ ls
events.bson  gridfs_data  job.json  job.log  queue_sub_script.sh
```

Check the batch script

Cryosparc batch script 수정

⑥ Adjust the number of ntasks in the batch script.

➤ \$ vim queue_sub_script.sh

[queue_sub_script.sh]

```
#!/bin/bash
#SBATCH --job-name=cryosparc_bmttest_P1_J5
#SBATCH --partition=mig-10gb
#SBATCH --output=/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5/job.log
#SBATCH --error=/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5/job.log
#SBATCH --gpus=2
#SBATCH --gres=gpu:2
#SBATCH --ntasks=4 → #SBATCH --ntasks=16
#SBATCH --cpus-per-task=1
```

```
export HOME=/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100
```

```
source $MODULESHOME/init/bash
```

```
module load cryosparc-bmttest/4.4.1-worker
```

```
/opt/cryoem/cryosparc-bmttest/4.4.1/cryosparc2_worker/bin/cryosparcw run --project P1 --job J5 --master_hostname olaf1 --master_command_core_port 41262 > /proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5/job.log 2>&1
```

Cryosparc batch script 수정

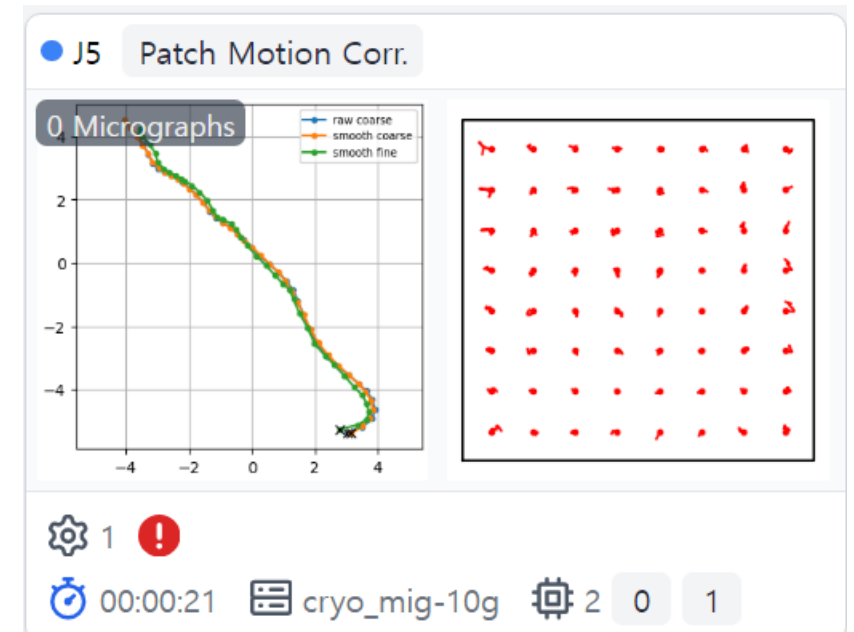
⑦ Submit the batch file.

- `$ sbatch queue_sub_script.sh`
Submitted batch job xxxxxxxx

⑧ Access the web and check the status (killed > Running).



※ It may take about 0-2 minutes to change to the Running status.



Notes

“memory per core” per partition

Core * Memory-Per-Core=[Total available memory allocated to the task]

ex) normal partition 12core allocate

Total memory=12*7.4=88.8G allocated

Partition Name	Node	Core	total-memory	memory-per-core
AIP	olaf-g[001-004]		1024G	16G
mig-1g.10gb	olaf-g012			
mig-1g.20gb	olaf-g[007-008,011]			
mig-3g.40gb	olaf-g[005-006,009-010]			
normal-cpu	olaf-c[001-210]	1	256G	none
long-cpu				
normal	olaf-cu[1-5]	1	768G	7.4G
long				
jepyc				
jepyc-rtx	jepyc50		64G	none
HQ2comp	HQ2comp[01-28]		48G	0.9G
HQcomp	HQcomp[01-28]		64G, 128G	2.2G
HQmem	HQmem[01-04]		64G	1.6G
			256G	12.5G

For inquiries, please contact us via email (ibs-cluster@ibs.re.kr)

A photograph of a forest with sunlight filtering through the trees, creating a warm and serene atmosphere. The sun is positioned in the upper center, casting long shadows and highlighting the textures of the tree trunks and the forest floor. The ground is covered in green moss and ferns. A semi-transparent white rounded rectangle is centered in the image, containing the text "Thank you." in a bold, black, sans-serif font.

Thank you.