



# Cryosparc sciprt 수정 방법

# Cryosparc log 분석

## ① 실패한 작업의 log 조사를 위해 경로 복사

The screenshot displays the CryoSPARC web interface. The top navigation bar shows the job name 'P1 BMT-10G-h100 W1 Data Processing J5 Patch Motion Correction' and a runtime of '49m 20s'. The main content area is divided into three sections:

- Event Log:** Shows a log entry for a failed job. 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 the grid, it indicates '1,120 exposures'.
- Micrographs incomplete:** A section showing '1,633 exposures' of incomplete micrographs.

On the right side, the 'Details' panel for job 'P1 J5 Patch Motion Correction' is visible. It shows the job title 'New Job J5', workspace 'W1', and status 'Failed'. The 'Directory' field is highlighted with a red box and contains the path: `/proj/home/ibs/bmttest/bmttest/shc/CS-bmt-10g-h100/J5`. A red arrow points from this box to the Korean text '클릭' (Click).

클릭

# Cryosparc log 분석

## ② 작업로그 조회

➤ `$ 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=11927000.batch. Some of your processes may have been killed by the cgroup out-of-memory handler.
```

OOM log 확인 시 core 수를 늘려서 작업을 돌려야 합니다.

# Cryosparc batch script 생성

③ 프로세싱된 데이터를 clear 해줍니다.

Details

Title New Job J5

Workspace W1

Tags No tags applied.

Status Failed

Created Apr 8, 2024, 10:09:15 AM

Created By Crayadmin Crayadmin

**ACTIONS**

- Queue Job
- Kill Job
- Clear 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
- Create Workflow

Actions View Job

2. Clear job

1. Actions

④ 작업 rebuild를 통해 작업을 submit 직후 killed 버튼을 통해 작업을 중지시킵니다.

Activity

Actions View Job

Queue

Cancel Queue

Activity

Actions View Job

3. Queue

4. Actions

5. kill job

Description.

스크립트 파일만을 남기기 위한 작업입니다.

Details

Title New Job J5

Workspace W1

Tags No tags applied.

Status Launched

Created Apr 8, 2024, 10:09:15 AM

Created By Crayadmin Crayadmin

**ACTIONS**

- Queue Job
- Kill Job**

# Cryosparc batch script 수정

⑤ 터미널 접속 후 해당 작업의 폴더로 이동합니다. (① 참조)

- \$ 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
```

batch 스크립트 확인

# Cryosparc batch script 수정

## ⑥ batch 스크립트에서 ntasks 수를 조정합니다.

➤ \$ 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

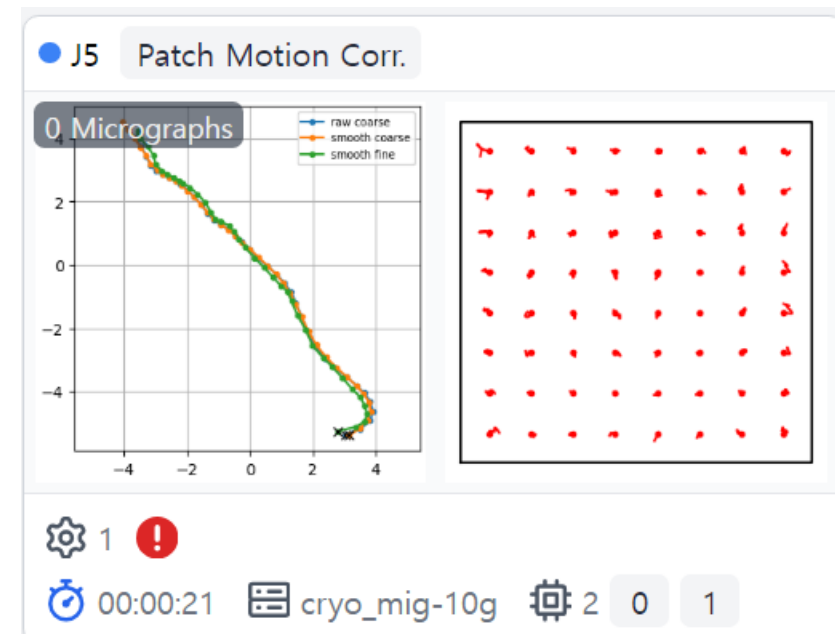
## ⑦ batch 파일 submit

- `$ sbatch queue_sub_script.sh`  
Submitted batch job 11928498

## ⑧ web 접속 후 Status 확인 (killed > Running)



※ Running 상태로 변경되기까지 0~2분 정도 소요될 수 있습니다.



# 참고사항

“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				
HQ2comp	HQ2comp[01-28]		64G, 128G	2.2G
HQcomp	HQcomp[01-28]		64G	1.6G
HQmem	HQmem[01-04]		256G	12.5G

문의 사항은 이메일(ibs-cluster@ibs.re.kr)이나 유선(878-9521)으로 연락 주시기 바랍니다 .



**감사합니다.**