

数据搬运与预处理使用说明

Titan#3 电镜数据的搬运：数据搬运

ssh preprocess@10.15.80.38 使用 preprocess 账户登录到相机的挂载节点

cd /Titan3_falcon/ 后，ls 看下今日的数据文件夹

cd /folder (例如：cd 20210913_wyx)进入到今日的数据存放文件夹。

```
12/10/2021 11:18.40 /home/mobaxterm ssh preprocess@10.15.80.38
preprocess@10.15.80.38's password:
Last login: Tue Oct 12 11:09:17 2021 from 10.15.56.106
[preprocess@pre_mgmt02 ~]$ cd /Titan3_falcon/
[preprocess@pre_mgmt02 Titan3_falcon]$ ls
20210913_wyx      20210926_HV      20210930_LF_tomo      20211004_M
20210915_zyl     20210928_test_2  20211001_mua_tomography_presets.xml  20211004_wjj
20210918_2_lkw  20210929_neron_7 20211003_M_1         Atlas-EPU
20210918_lkw    20210929_neron_8 20211003_wjj         EER_test
[preprocess@pre_mgmt02 Titan3_falcon]$ cd 20210913_wyx
```

ls 确认有一个.gain 背底文件在此文件夹内 (如: 20210909_142922_EER_GainReference.gain)。如果没有，通过电镜 PC 的桌面快捷链接 (EF-Falcon Reference)，复制一份.gain 背底文件至今日的数据存放文件夹，(如 Z:\20210913_wyx\)

确认有图片生成以后开始启动下面的搬运程序。

/home/script/eer.pl, 将引号内的 example 拷贝下来并根据例子进行更改

```
preprocess@10.15.80.38's password:
Last login: Tue Oct 12 11:09:17 2021 from 10.15.56.106
[preprocess@pre_mgmt02 ~]$ cd /Titan3_falcon/
[preprocess@pre_mgmt02 Titan3_falcon]$ ls
20210913_wyx      20210926_HV      20210930_LF_tomo      20211004_M      EER_test_back      gain_20211002      gain3.mrc      gain_post_ec.mrc      MRC_test      TIA
20210915_zyl     20210928_test_2  20211001_mua_tomography_presets.xml  20211004_wjj    gain_20210824      gain_20211004      gain3.mrc-      HealthMonitoring.db      MRC_test_back      Tomo_Data
20210918_2_lkw  20210929_neron_7 20211003_M_1         Atlas-EPU      gain_20210909      gain2.mrc      gain_2       ImagesForProcessing      SensorDefects.xml      Tomography_software
20210918_lkw    20210929_neron_8 20211003_wjj         EER_test      gain_20210929      gain2.mrc-      gain.mrc      makeEerGain.py      Supervisor_20210928_training-appof
[preprocess@pre_mgmt02 Titan3_falcon]$ cd 20210913_wyx
[preprocess@pre_mgmt02 20210913_wyx]$ ls
20210909_142922_EER_GainReference.gain  20210909_142922_EER_GainReference.gain.txt  EpuSession.dm  gain_normal.raw  gain_normal.raw.txt  gain_post_ec.raw  gain_post_ec.raw.txt  Images-Disc1  Metadata
[preprocess@pre_mgmt02 20210913_wyx]$ /home/script/Falcon_EER.pl
Usage: /home/script/Falcon_EER.pl
-scope_name the name of Microscope, e.g. Titan1,Titan2,Titan3,Arctica
-user_name: the name of user dir, e.g. liuzhj
-group_name the group of the user
-dir under user dir what folder user would like to store the data, e.g. 20181115_huattan
-ori_folder the folder name you want to process, e.g. supervisor_20181010_135940
-job the stack name you want to change to, e.g. abc
-raw_num next image number would like to change to. For a new folder, it should be 1
(-option)
-drive_space up to what percentage users' hard drive prefer to fill, default 90%
input: example: tmux new -d -s Falcon_EER -b tmux send -t Falcon_EER 'sudo /home/script/Falcon_EER.pl -scope_name Titan3 -user_name liuzhj -group_name liuzhj -ori_folder 20181121_HT -dir 20181115_huattan -job abc -raw_num 1' ENTER
to end the script, enter: tmux kill-session -t Falcon_EPU
to view whether the script is ended, enter: tmux ls
[preprocess@pre_mgmt02 20210913_wyx]$ sudo /home/script/Falcon_EER.pl -scope_name Titan3 -user_name liuzhj -group_name liuzhj -ori_folder 20210913_wyx -dir 20210913_wyx_1 -job 20210913_wyx_1 -raw_num 1
[sudo] password for preprocess:
```

示例：`sudo /home/script/eer.pl -scope_name Titan3 -user_name liuzhj -group_name liuzhj -ori_folder 20210913_wyx -dir 20210913_wyx -job 20210913_wyx -raw_num 1`

注意：`-ori_folder` 搬运前文件夹名字，`-dir` 参数表示搬运后目标文件夹名字，`-job` 参数表示搬运后目标文件名字，建议命名采用统一的格式，即日期_用户姓名标识 (如 20210913_wyx)，括号内容可选。

➤ Ctrl+C 数据搬运的停止

2 数据预处理

ssh user_name@10.15.80.45 以搬运脚本专用课题组账户(如: ssh liuzhj@10.15.80.45)登录预处理节点一。后备节点二: 10.15.80.46

cd EM_data/folder (例如: cd EM_data/20210913_wyx) 进入到搬运过来对应的文件夹位置, ls 下确定搬过来以后再开始预处理

```
12/10/2021 11:23:15 /home/mobaxterm ssh liuzhj@10.15.80.45
Warning: Permanently added '10.15.80.45' (RSA) to the list of known hosts.
liuzhj@10.15.80.45's password:
Last login: Sat Aug 21 16:25:31 2021 from 10.15.81.228
[liuzhj@pre-gpu-b-node01 ~]$ ls
EM_data
[liuzhj@pre-gpu-b-node01 ~]$ cd EM_data/
[liuzhj@pre-gpu-b-node01 EM_data]$ ls
20210902_wyx 20210903_lkw 20210909_zjy 20210913_wyx 20210914_ch 20210916_lkw 20210918_lkw 20210923_wyx 202
20210902_wyx1 20210904_lkw 20210913_ch 20210913_wyx_1 20210915_zyl 20210917_wt 20210918_wt 20210924_ch 202
[liuzhj@pre-gpu-b-node01 EM_data]$ cd 20210913_wyx_1
[liuzhj@pre-gpu-b-node01 20210913_wyx_1]$ ls
20210909_142922_EER_GainReference.gain 20210913_wyx_1 20210913_wyx_1_0001.tan 20210913_wyx_1_0002.eer
20210909_142922_EER_GainReference.gain.txt 20210913_wyx_1_0001.eer 20210913_wyx_1_0001.xml 20210913_wyx_1_0002.tan
```

ps au 预处理开始前需要看下该节点是不是还有其他未处理完成的进程, 如有则需要 kill 掉, 如果没有多余进程(如下图)则无需 kill, 可以进行下一步操作。

```
[sunqq@pre-gpu-b-node01 ~]$ ps au
USER      PID %CPU %MEM    VSZ   RSS TTY      STAT START   TIME COMMAND
root         3612  0.0  0.0 110088   856 tty1      Ss+   Aug06    0:00 /sbin/agetty --noclear tty1 li
sunqq     22590  0.0  0.0 120864  3412 pts/1    Ss   13:45    0:00 -bash
raozh     42019  0.0  0.0 120908  3548 pts/0    Ss+  10:18    0:00 -bash
sunqq     45635  0.0  0.0 159580  2012 pts/1    R+   13:48    0:00 ps au
```

/home/script/Titan3/Titan3_eer.pl 根据提示并根据例子进行更改。

```
liuzhj@pre-gpu-b-node01 20210913_wyx_1]$ /home/script/Titan3/Titan3_eer.pl
Usage /home/script/Titan3/Titan3_eer.pl
-mode 1:counting 2:super resolution
-user user_name
-job job_name
-raw_f raw_image folder
-raw_n rename start number
-psize Pixel size
-total_dose total dose of the stack in unit of e/A2
[option] Default Introduction
-av 300.0 Acceleration voltage
-spc 2.7 Spherical aberration
-ac 0.07 Amplitude contrast
-sps 512 Size of power spectrum to compute
-min_r 30.0 Minimum resolution
-max_r 5.0 Maximum resolution
-min_d 5000.0 Minimum defocus
-max_d 50000.0 Maximum defocus
-dss 500 Defocus search step
-exa 1000 Expected (tolerated) astigmatism
-phase yes Find additional phase shift? 1: yes; 2: no
-min_Pshift 0.0 Minimum phase shift (rad)
-max_Pshift 3.15 Minimum phase shift (rad)
-PS_step 0.5 Phase shift search step
-drive space 90% up to how many percentage user's hard drive prefer to fill
-stack_size the file size of mrcs stack (e.g.2080375808)

super resolution mode example: /home/script/Titan3/Titan3_eer.pl -mode 2 -user liuzhj -job F4 -raw_f 20190111_huatian -raw_n 1 -psize 0.52 -total_dose 50
super resolution mode with phase plate example: /home/script/Titan3/Titan3_eer.pl -mode 2 -user liuzhj -job F4 -raw_f 20190111_huatian -raw_n 1 -psize 0.52 -total_dose 50 -phase 1
liuzhj@pre-gpu-b-node01 20210913_wyx_1]$ /home/script/Titan3/Titan3_eer.pl -mode 2 -user liuzhj -job 20210913_wyx_1 -raw_f 20210913_wyx_1 -raw_n 1 -psize 0.75 -total_dose 60
```

例: /home/script/Titan3/Titan3_eer.pl -mode 2 -user liuzhj -job 20210913_wyx -raw_f 20210913_wyx -raw_n 1 -psize 0.96 -total_dose 60

注意: -user 为用户名 搬运前文件夹名字, -job 参数表示需要处理的目标文件名, -raw_f 参数表示需要处理的目标文件名字, -raw_n 起始处理的数字编号, -psize

为收数据使用的 pixel size 大小, -total_dose 为总剂量。

➤ 查看图片预处理结果的相关信息 (查看的停止均为 Ctrl+C):

用 username 登录到对应的预处理节点, 进入到预处理的文件夹

1) tail -f filename (如: tail -f 20210901_coma_test)

```
[sunqq@pre-gpu-b-node01 20210901_coma_test]$ tail -f 20210901_coma_test
29287.296 1342214144 1630477874 20210901_coma_test_0001 6794.056 6726.568 67.49 84.047 0.277 4.685 12% 4.71 2021-09-01 14:31 0.00 40
29139.234 1342214144 1630477884 20210901_coma_test_0002 8252.650 8172.757 79.89 87.310 0.266 4.625 12% 3.09 2021-09-01 14:31 0.00 40
29379.925 1342214144 1630477860 20210901_coma_test_0003 4661.354 4578.924 82.43 83.938 0.262 4.685 12% 4.31 2021-09-01 14:31 0.00 40
29561.727 1342214144 1630477894 20210901_coma_test_0004 5035.086 5035.086 0.00 34.183 0.319 4.747 12% 4.74 2021-09-01 14:31 0.00 40
28905.662 1342214144 1630477905 20210901_coma_test_0005 5711.546 5637.759 73.79 83.601 0.275 4.747 12% 3.46 2021-09-01 14:31 0.00 40
28939.059 1342214144 1630477915 20210901_coma_test_0006 8308.137 8228.825 79.31 -82.635 0.244 4.537 12% 3.53 2021-09-01 14:31 0.00 40
29487.569 1342214144 1630477926 20210901_coma_test_0007 41701.102 41581.570 119.53 -5.268 0.036 10.096 12% 4.84 2021-09-01 14:32 0.00 40
26611.211 1342214144 1630477936 20210901_coma_test_0008 6358.537 6305.848 52.69 81.960 0.257 4.625 12% 4.22 2021-09-01 14:32 0.00 40
29217.562 1342214144 1630477946 20210901_coma_test_0009 7568.101 7509.744 58.36 -84.920 0.241 4.625 12% 4.86 2021-09-01 14:32 0.00 40
29072.953 1342214144 1630477957 20210901_coma_test_0010 7086.784 6965.503 121.28 80.355 -0.030 716.800 12% 4.9 2021-09-01 14:32 0.00 40
```

2) tail -f filename_TEMstigma (可根据推荐值直接调节电镜的物镜像散)

注意: 三号机的像散推荐值用法, 如预处理的均值 $x = 0.00010, y = -0.00010$, 则在电镜调节物镜像散 $x - 0.00010, y + 0.00010$ 。

```
[sunqq@pre-gpu-b-node01 20210901_coma_test]$ tail -f 20210901_coma_test_TEMstigma
20210901_coma_test_0001: 0.00014,-0.00012
20210901_coma_test_0002: 0.00015,-0.00010
20210901_coma_test_0003: 0.00017,-0.00015
20210901_coma_test_0004: 0.00000,0.00000
20210901_coma_test_0005: 0.00015,-0.00013
20210901_coma_test_0006: 0.00008,-0.00020
20210901_coma_test_0007: -0.00024,0.00022
20210901_coma_test_0008: 0.00012,-0.00009
20210901_coma_test_0009: 0.00007,-0.00014
20210901_coma_test_0010: 0.00028,-0.00018
```

3) dosef_logviewer 在弹出窗口输入 filename_####_imod_Log.txt 即可查看

```
[sunqq@pre-gpu-b-node01 20210901_coma_test]$ dosef_logviewer
```

