

数据搬运与预处理使用说明

Titan#3 电镜数据的搬运

纯手动例：`rsync -avP -e 'ssh -p 10086' /Titan3_falcon/20210913_wangyinxian/* liuzhj@10.15.56.142:/home/liuzhj/EM_data/20210913_wangyinxian/`

1. `ssh preprocess@10.15.80.49` 使用 `preprocess` 账户登录到相机的挂载节点
2. `cd /Titan3_falcon/` 后，`ls` 看下今日的数据文件夹
3. `cd /folder` (例如：`cd 20210913_wangyinxian`)进入到今日的数据存放文件夹。

```

preprocess@10.15.80.49 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_wangyinxian      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_wangyinxian
  
```

4. `ls` 通过电镜 PC 的桌面快捷链接 (EF-Falcon Reference)，复制所有背底文件至今日的数据存放文件夹，(如 `Z:\20210913_wangyinxian\`)。
5. `/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  20210928_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_135840
-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's hard drive prefer to fill, default 90%
input example: tmux new -d -s Falcon_EER -d 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_wangyinxian -dir 20210913_wangyinxian -job 20210913_wangyinxian -raw_num 1`

注意：默认 (`-user_name` 和 `-group_name`) 统一用课题组账户名(如 `liuzhj`)。默认 (`-ori_folder` 和 `-dir` 和 `-job`) 统一，即日期_用户姓名 (如 `20210913_wangyinxian`)。

`-ori_folder` 搬运前文件夹名，`-dir` 表示搬运后目标文件夹名，`-job` 参数表示提交任务名。以上会生成并搬到新路径 `/home/liuzhj/EM_data/20210913_wangyinxian`。

6. `Ctrl+C` 数据搬运停止。

数据预处理

7. `ssh user_name@10.15.80.47` 以课题组账户(如: `ssh liuzhj@10.15.80.47`)登录预处理节点一。后备节点二: 10.15.80.44。(.80.47 = Titan3a ; .80.44 = Titan3b)
8. `cd EM_data/folder` (例如: `cd EM_data/20210913_wangyinxian`) 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

```

9. `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

```

10. `/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
-acv 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_mrccs_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_wangyinxian -raw_f 20210913_wangyinxian -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字, `-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。

查看预处理结果

12. 开启新窗口三个，重复步骤 7 和 8 三次，分别进入到预处理的文件夹

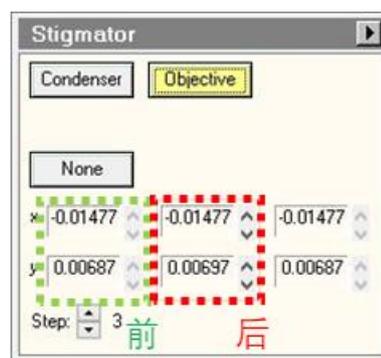
13. 窗口一，`tail -f filename`（如：`tail -f 20210901_coma_test`）

```
[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
29551.727      1342214144      1630477894      20210901_coma_test_0004 5035.006      5035.006      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
```

14. 窗口二，`tail -f filename_TEMStigma`（可根据推荐值直接调节电镜的物镜像散）

注意：三号机的像散修正方法，如下左，预处理的均值 ($x \sim 0$), ($y \sim -0.00010$), 如右图调节物镜像散 (x 有正负不用调), ($y + 0.00010$)。

```
[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,-0.00016
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
```



15. 窗口三，`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
```

