UT Southwestern Medical Center
Lyda Hill Department of Bioinformatics

BioHPC

Introduce of CryoEM Resources on BioHPC

[web] portal.biohpc.swmed.edu
[email] biohpc-help@utsouthwestern.edu

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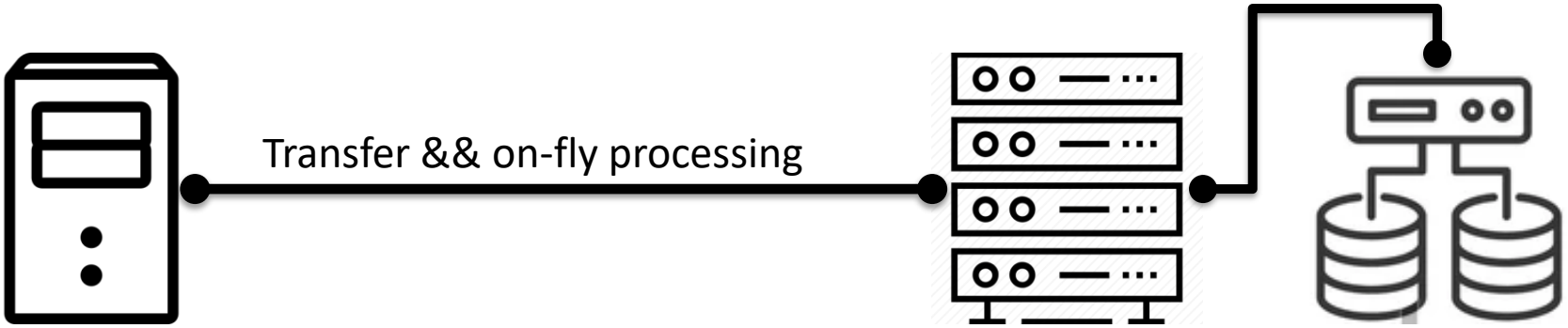
Overview CryoEM resources on BioHPC

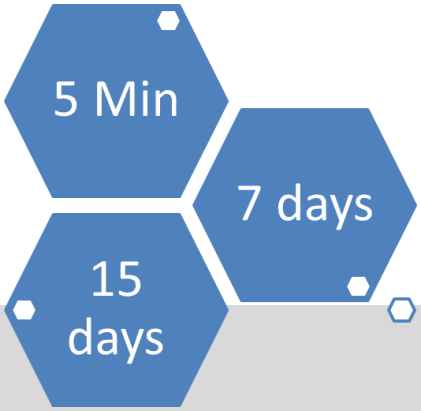
- **Raw image transfer and on-fly processing, Data Storage**
- **Web Visualization, Interactive job, SLURM job**
- **BioHPC workstation**
- **GPU partitions:**
  - >100 nodes Nvidia - Tesla K20/K40, P4, P40, P100, V100s, 4V100, A100, more will come.
- **Tools:**
  - RELION, cryoSPARC, EMAN2, MotionCorr, Coot, Cryolo, Chimera, IMOD, PEET, SBGrid, et.al.

Data transfer and Storage



Camera PCs

:\DoseFraction\<**user**>\Images-Disc
:\DoseFraction\<**user**>\KEEP



BioHPC cluster and storage

/project/cryoem/cryoem_transfer/<**krios**>/<**user**>
…
…
…

Important: Move to your own space on BioHPC or local server after your cryoEM microscope session.

Access data storage on BioHPC

As a BioHPC user, you will have several storage options:

BioHPC Standard Storage Limits

/home2/<username>	50 GB per user
/work/<department>/<username>	5 TB per user
/project/<organization>/<group>/<username>	5 TB per group
/archive/<organization>/<group>/<username>	5 TB per group

BioHPC File Exchange (accessible to outside of UTSW)

https://cloud.biohpc.swmed.edu 50 GB / user

BioHPC Lamella Cloud Storage (UTSW-only)

https://lamella.biohpc.swmed.edu 100 GB / user
(FTP, SAMBA or WebDAV*)

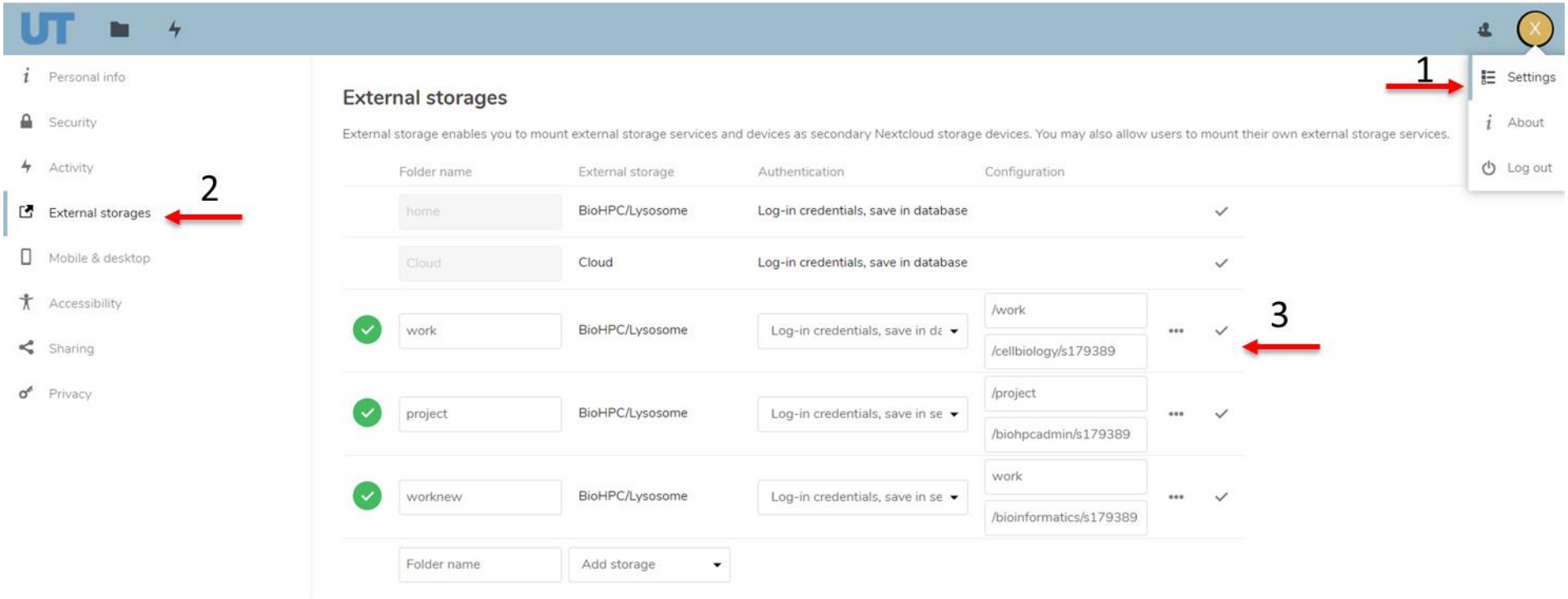
Project and Archive can be increased on PI request with Dept. Chair approval.
Archive usage is multiplied by 2/3 (as to encourage use of archive).
Data on home2 counts thrice and on work counts twice because of backup.

Guides about BioHPC storage:

1, BioHPC portal Guides/FAQ pages: BioHPC Guides (swmed.edu)

2, BioHPC training slides: BioHPC Storage Overview (swmed.edu)

Setting up Lamella to access project and work space



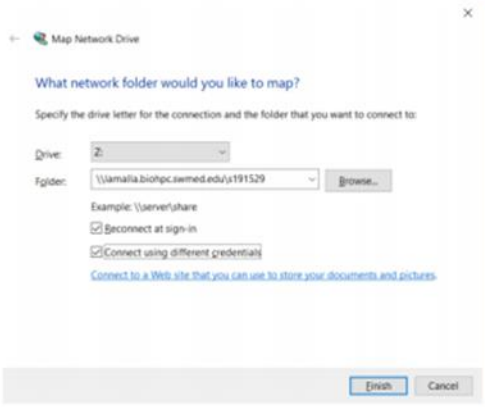
Setting up Lamella to access project and work

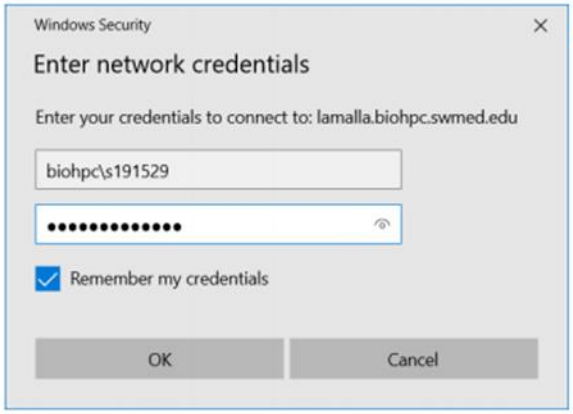
Computer -> Map Network Drive

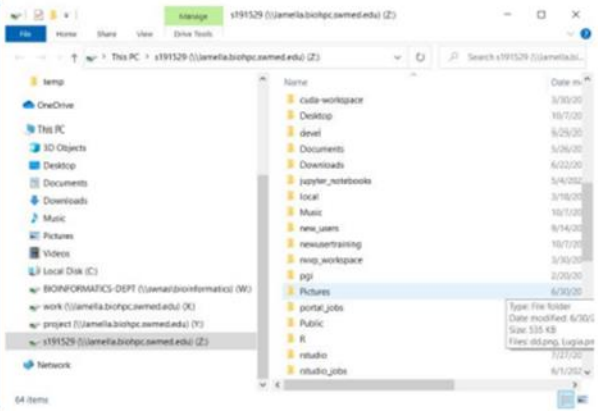
Folder is: \\lamella.biohpc.swmed.edu*username* *(home dir)*
\\lamella.biohpc.swmed.edu\project
\\lamella.biohpc.swmed.edu\work

Check 'Connect using different credentials'

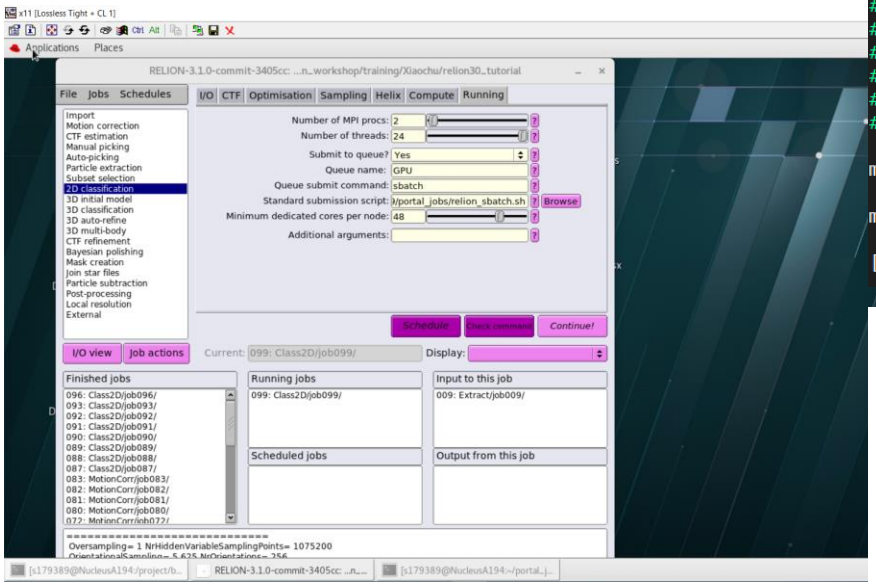
Enter your BioHPC username and password when prompted.

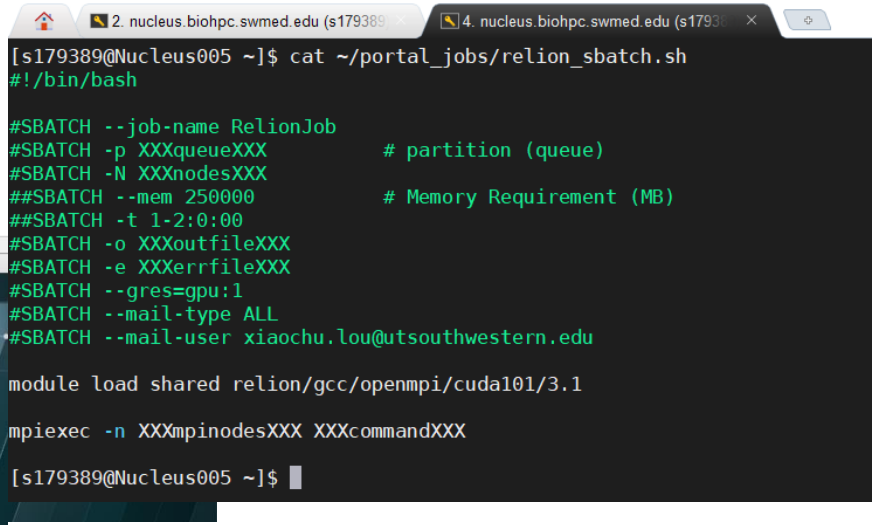


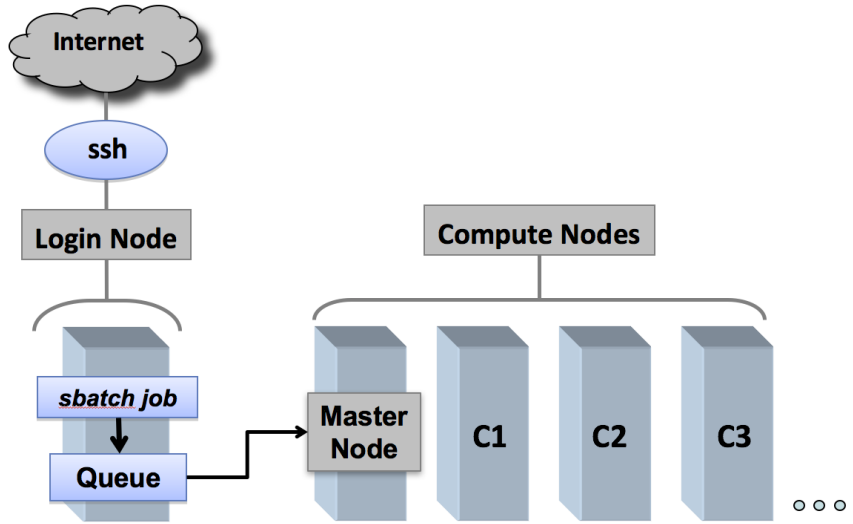




Web Visualization and Slurm Job







GPU nodes

GPU Partition	Number of CPU/Node	Memory Per Node	Number of GPU/Node	GPU Memory	Number of nodes
GPU	32	256GB	1 K20/K40	6GB/12GB	8
GPUp4	72	384GB	1 P4	8GB	16
GPUp40	72	384GB	1 P40	24GB	16
GPUp100	56	256GB	2 P100	16GB	12
GPUv100s	72	384GB	1 V100S	32GB	32
GPU4v100	72	384GB	4 V100S	32GB	12
GPUA100	72	1.5TB	1 A100	40GB	16
GPU4A100	72	1.5TB	4 A100	80GB	10

Check node availability

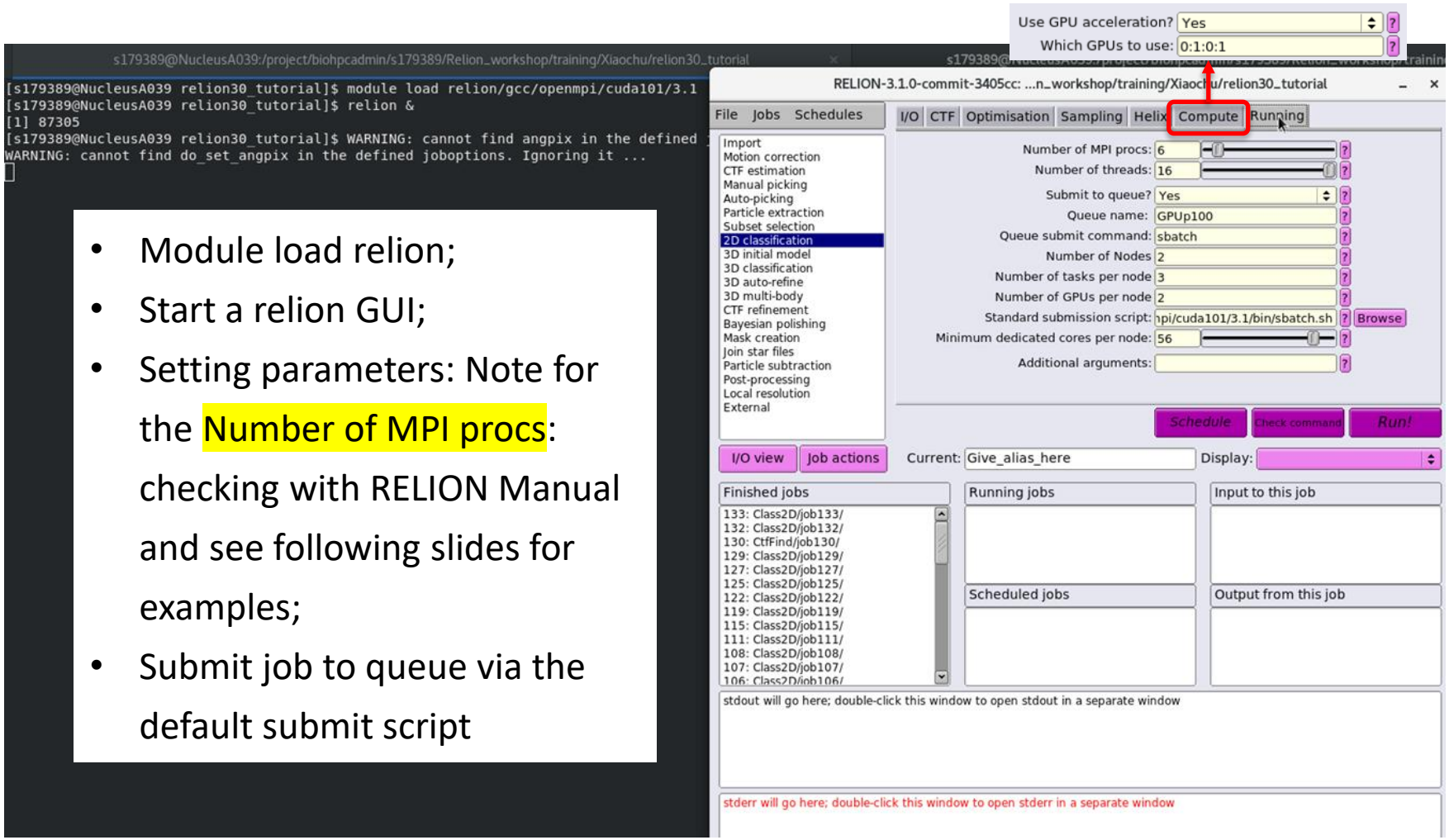
```
[s179389@Nucleus005 ~]$ sinfo -p GPUp4
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
GPUp4        up   infinite      5  alloc NucleusC[002,012-013,016-017]
GPUp4        up   infinite     11   idle NucleusC[003-011,014-015]
```

Modules

```
[s179389@Nucleus005 ~]$ module avail

------------------------------------------------------------ /cm/local/modulefiles ------------------------------
cluster-tools/7.3 dot             gcc/6.1.0        module-git       null             shared
cmd               freeipmi/1.5.2  ipmitool/1.8.17  module-info      openldap         use.own

------------------------------------------------------------ /cm/shared/modulefiles -----------------------------
abra2/2.18                                  intel/mkl/32/2017/6.256
acml/gcc/64/5.3.1                           intel/mkl/64/2017/6.256
acml/gcc/fma4/5.3.1                         intel/mkl/64/2017/current
acml/gcc/mp/64/5.3.1                        intel/mkl/mic/2017/6.256
acml/gcc/mp/fma4/5.3.1                      intel/mpi/32/2017/6.256
acml/gcc-int64/64/5.3.1                     intel/mpi/64/2017/6.256
acml/gcc-int64/fma4/5.3.1                   intel/mpi/mic/2017/6.256
acml/gcc-int64/mp/64/5.3.1                  intel-cluster-checker/2.1.2
acml/gcc-int64/mp/fma4/5.3.1                intel-cluster-runtime/ia32/3.8
afni/20.0.04                                intel-cluster-runtime/intel64/3.8
afni/v17.2.17                               intel-cluster-runtime/mic/3.8
afni/v18.3.03                               intel-tbb-oss/ia32/2017_20170807oss
almost/2.1                                  intel-tbb-oss/intel64/2017_20170807oss
amber/12                                    io_lib/1.13.3
```

```
[s179389@Nucleus005 ~]$ module avail relion

------------------------------------------------------------ /cm/shared/modulefiles -----------------------------
relion/gcc/1.2                      relion/gcc/openmpi/cuda80/2.0-beta    relion/intel/openmpi/1.4
relion/gcc/1.3                      relion/gcc/openmpi/cuda80/2.1.0       relion/intel/openmpi/cuda101/3.1-beta
relion/gcc/mvapich2/1.4             relion/gcc/openmpi/cuda91/2.1.0       relion/intel/openmpi/cuda80/2.0-beta
relion/gcc/openmpi/1.4              relion/intel/1.3                      relion/intel/openmpi/cuda91/3.0.1
relion/gcc/openmpi/cuda101/3.1      relion/intel/mvapich2/1.4
[s179389@Nucleus005 ~]$ module avail cryosparc

------------------------------------------------------------ /cm/shared/modulefiles -----------------------------
cryosparc/2.15.0-6-singularity cryosparc/3.1.0-singularity
[s179389@Nucleus005 ~]$ module avail imod

------------------------------------------------------------ /cm/shared/modulefiles -----------------------------
imod/4.7.5            imod/4.8.50-beta       imod/cuda65/4.8.50-beta imod/cuda80/4.11.0      imod/cuda80/4.9.3
imod/4.8.38           imod/4.9.3             imod/cuda80/4.10.32     imod/cuda80/4.9.12
[s179389@Nucleus005 ~]$
```

Run RELION and submit RELION batch job for GPU intensive jobs



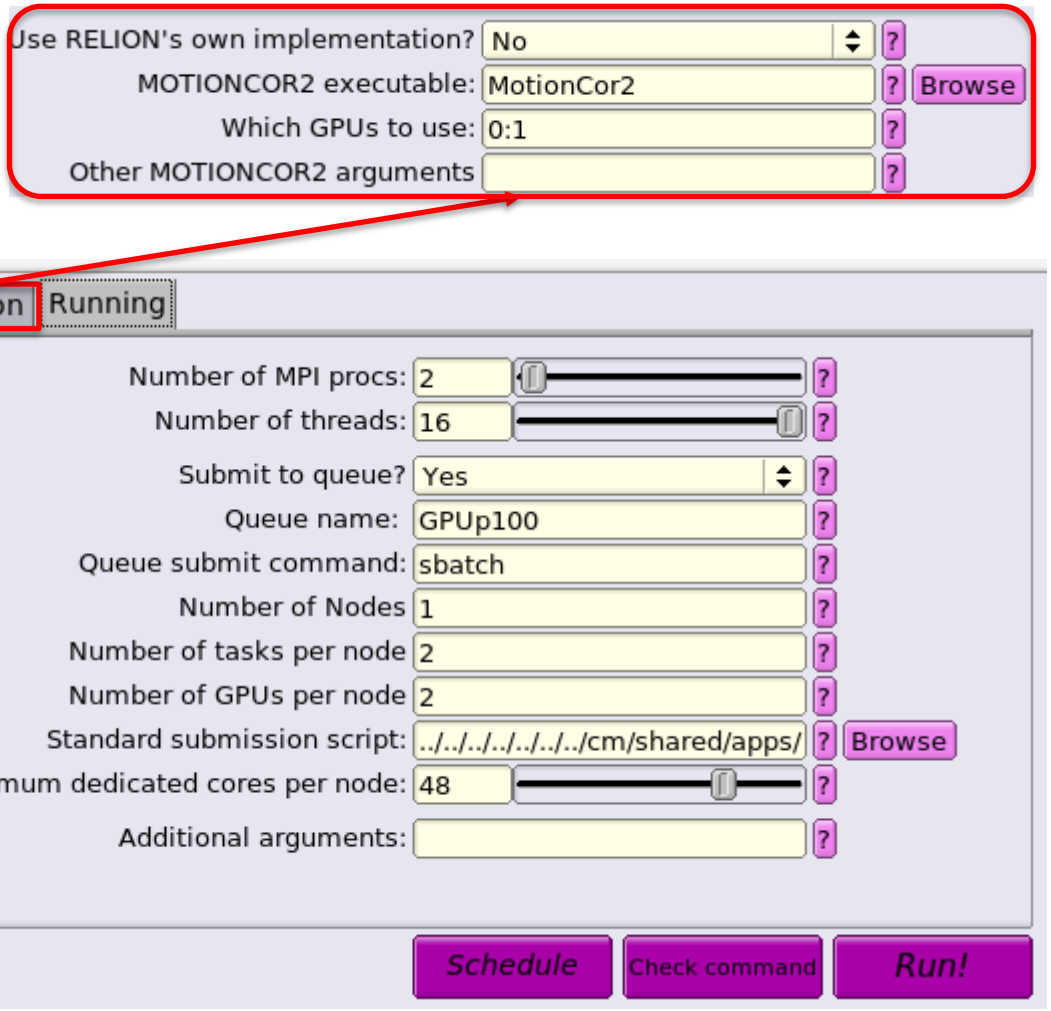
- Module load relion;
- Start a relion GUI;
- Setting parameters: Note for the Number of MPI procs: checking with RELION Manual and see following slides for examples;
- Submit job to queue via the default submit script

Examples of submitting RELION job to multiple nodes

Motion correction

1 GPUp100 nodes,

2 GPU cards on each nodes

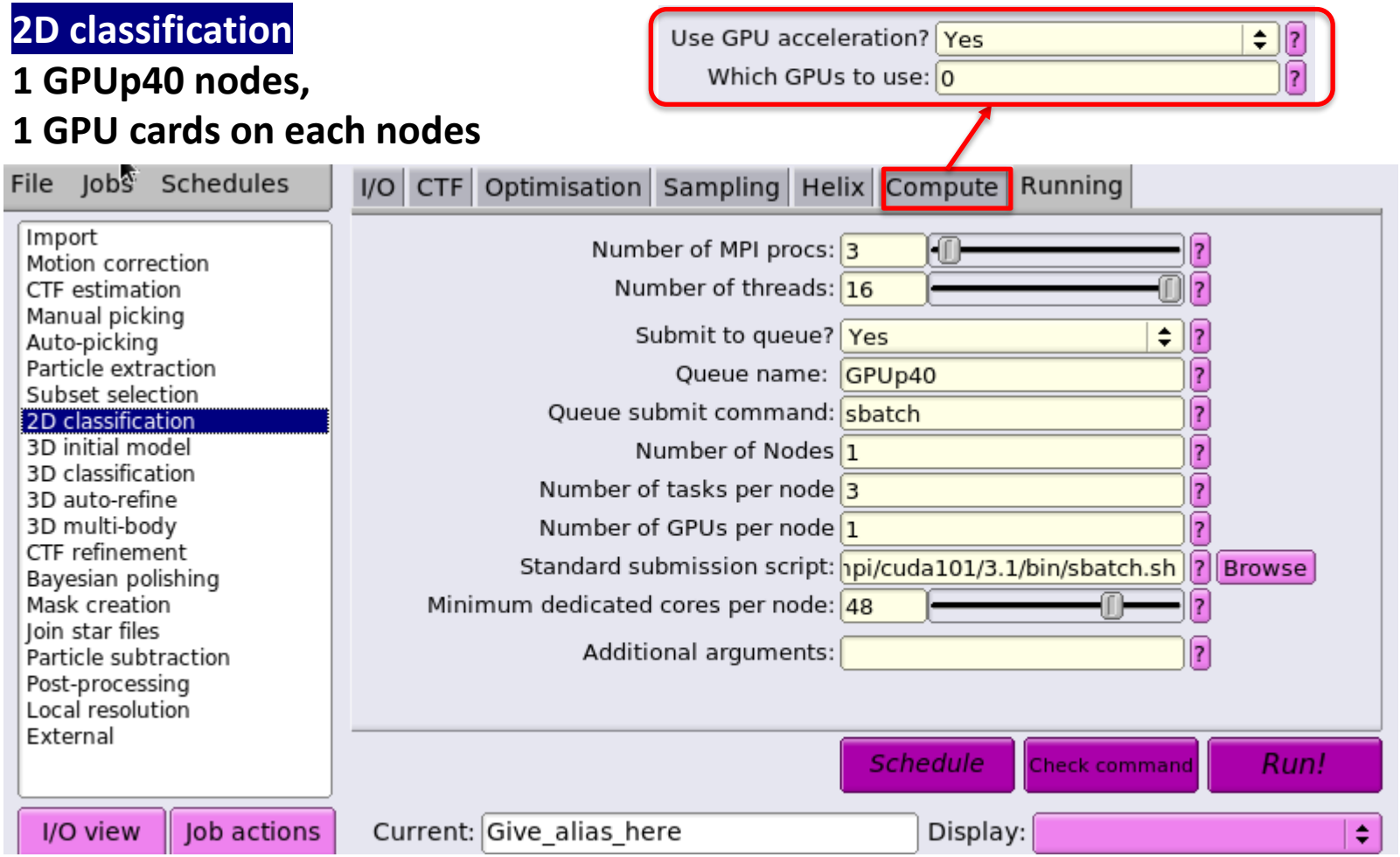


Examples of submitting RELION job to multiple nodes

2D classification

1 GPUp40 nodes,

1 GPU cards on each nodes

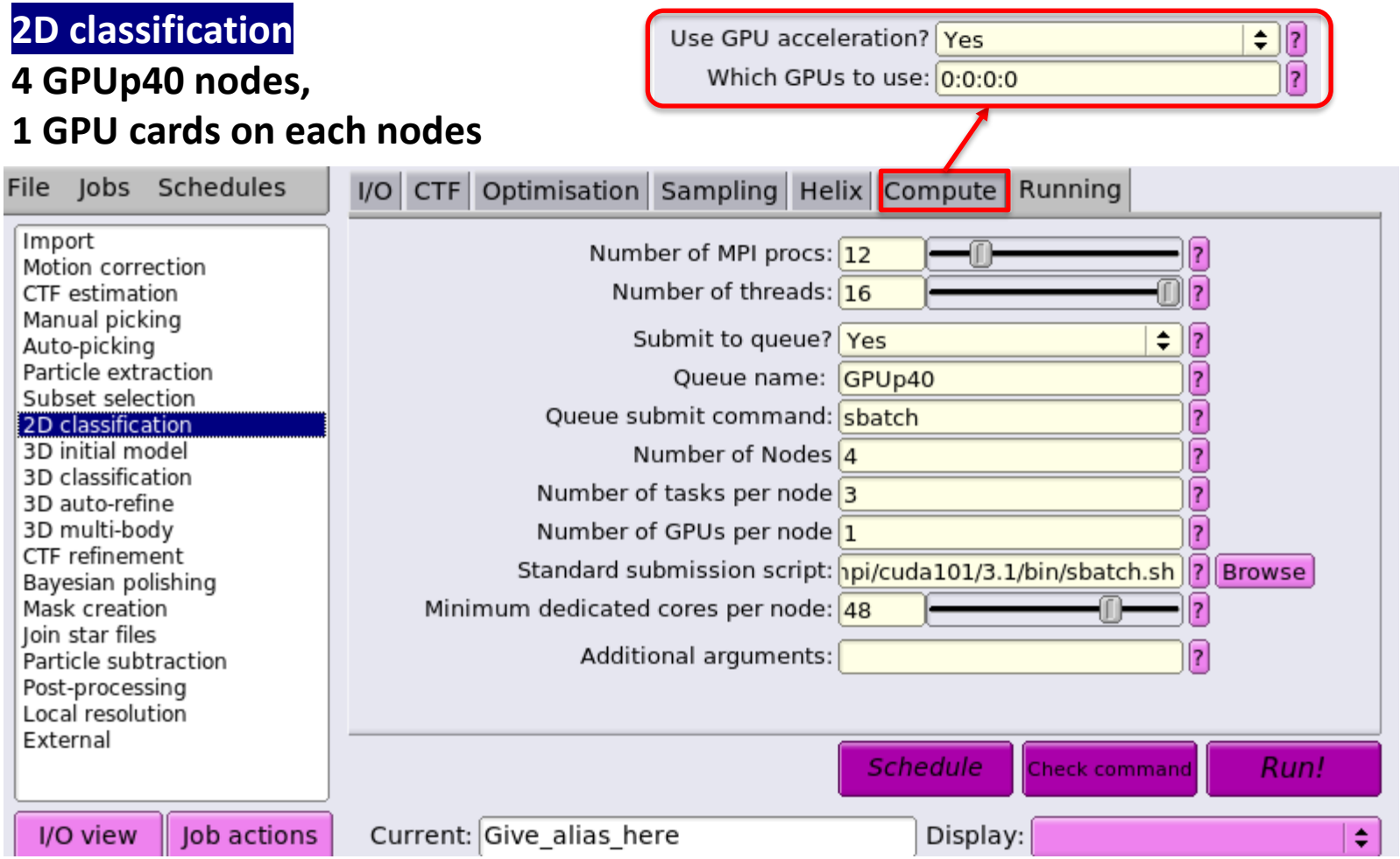


Examples of submitting RELION job to multiple nodes

2D classification

4 GPUp40 nodes,

1 GPU cards on each nodes

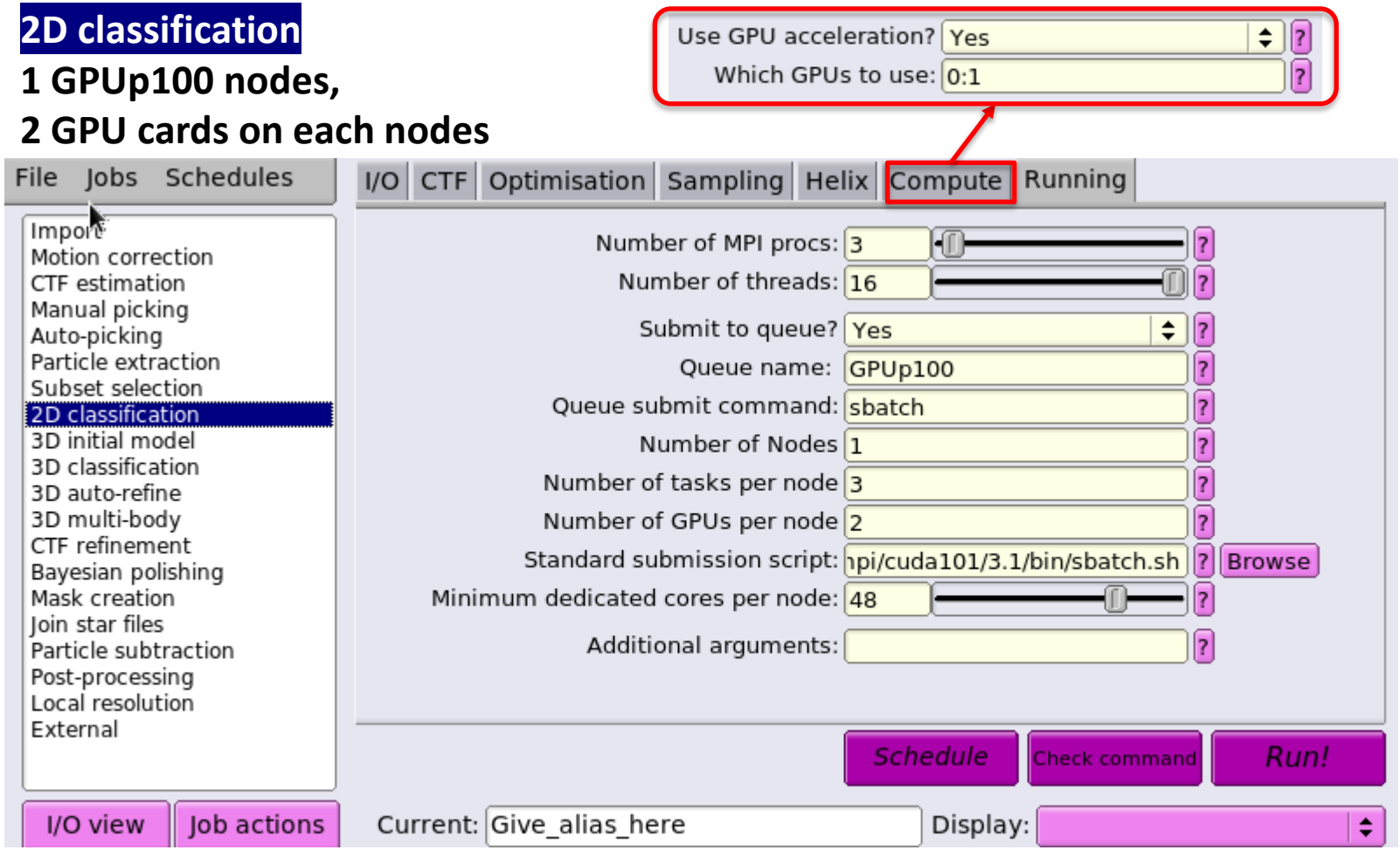


Examples of submitting RELION job to multiple nodes

2D classification

1 GPUp100 nodes,

2 GPU cards on each nodes

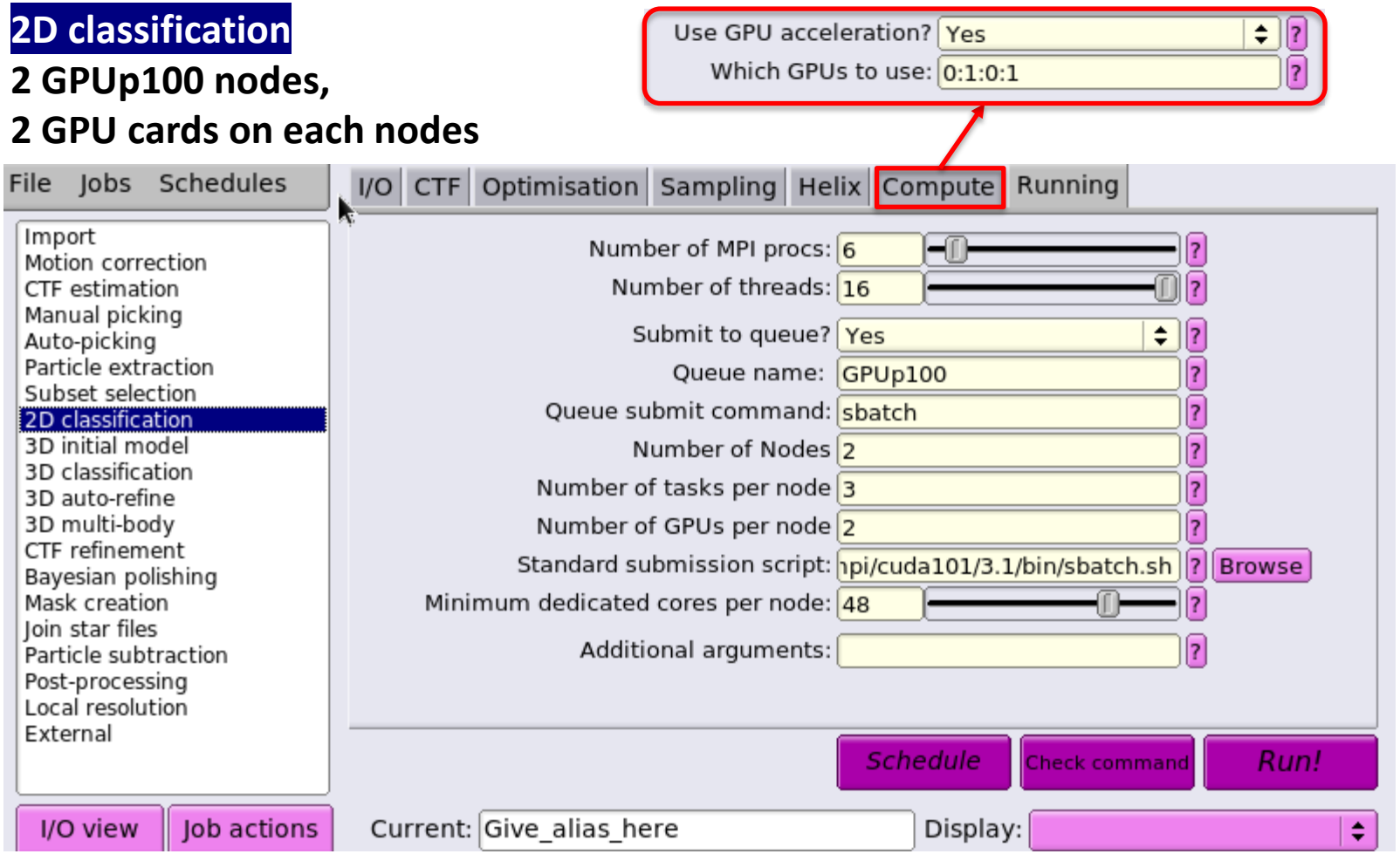


Examples of submitting RELION job to multiple nodes

2D classification

2 GPUp100 nodes,

2 GPU cards on each nodes

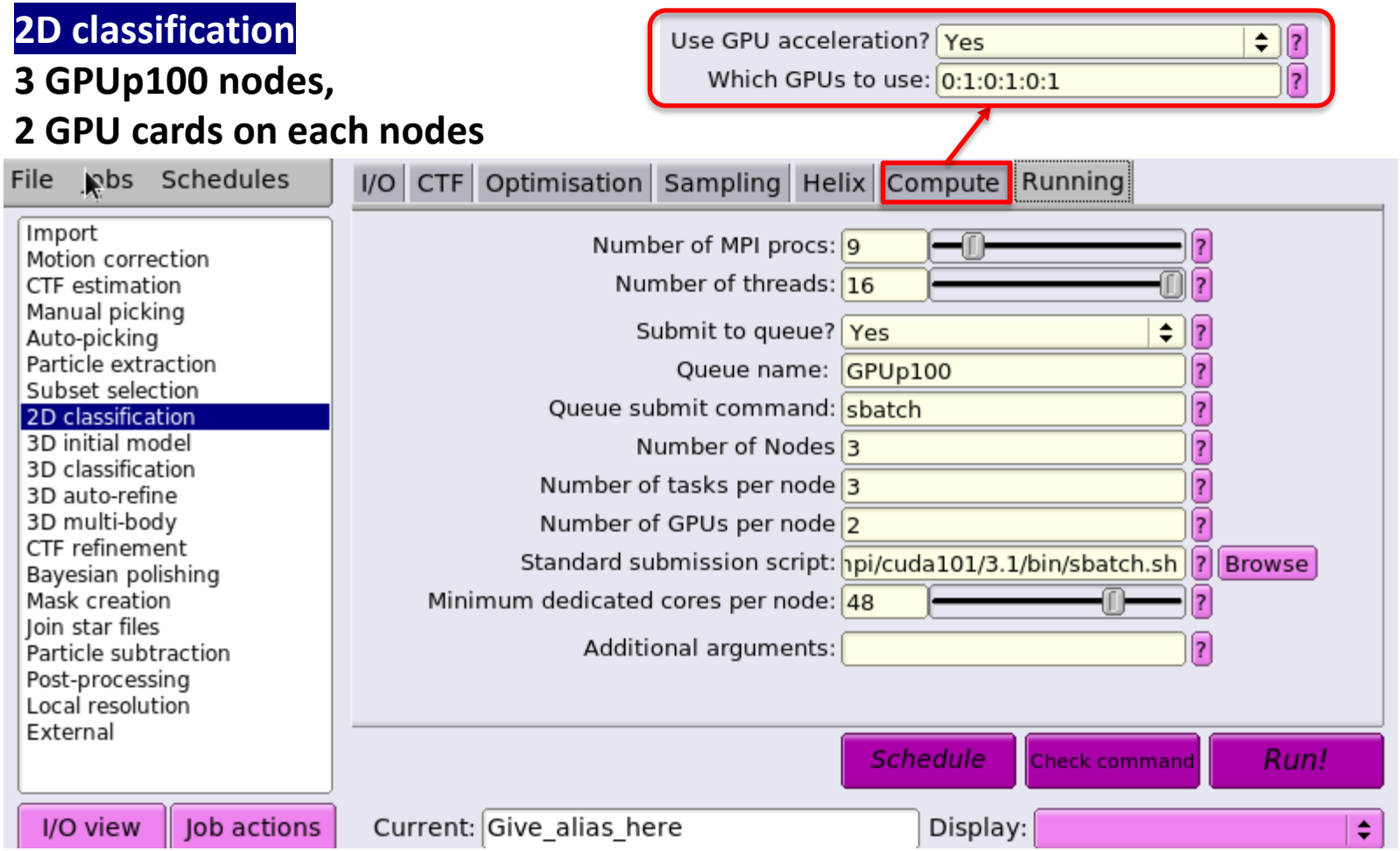


Examples of submitting RELION job to multiple nodes

2D classification

3 GPUp100 nodes,

2 GPU cards on each nodes

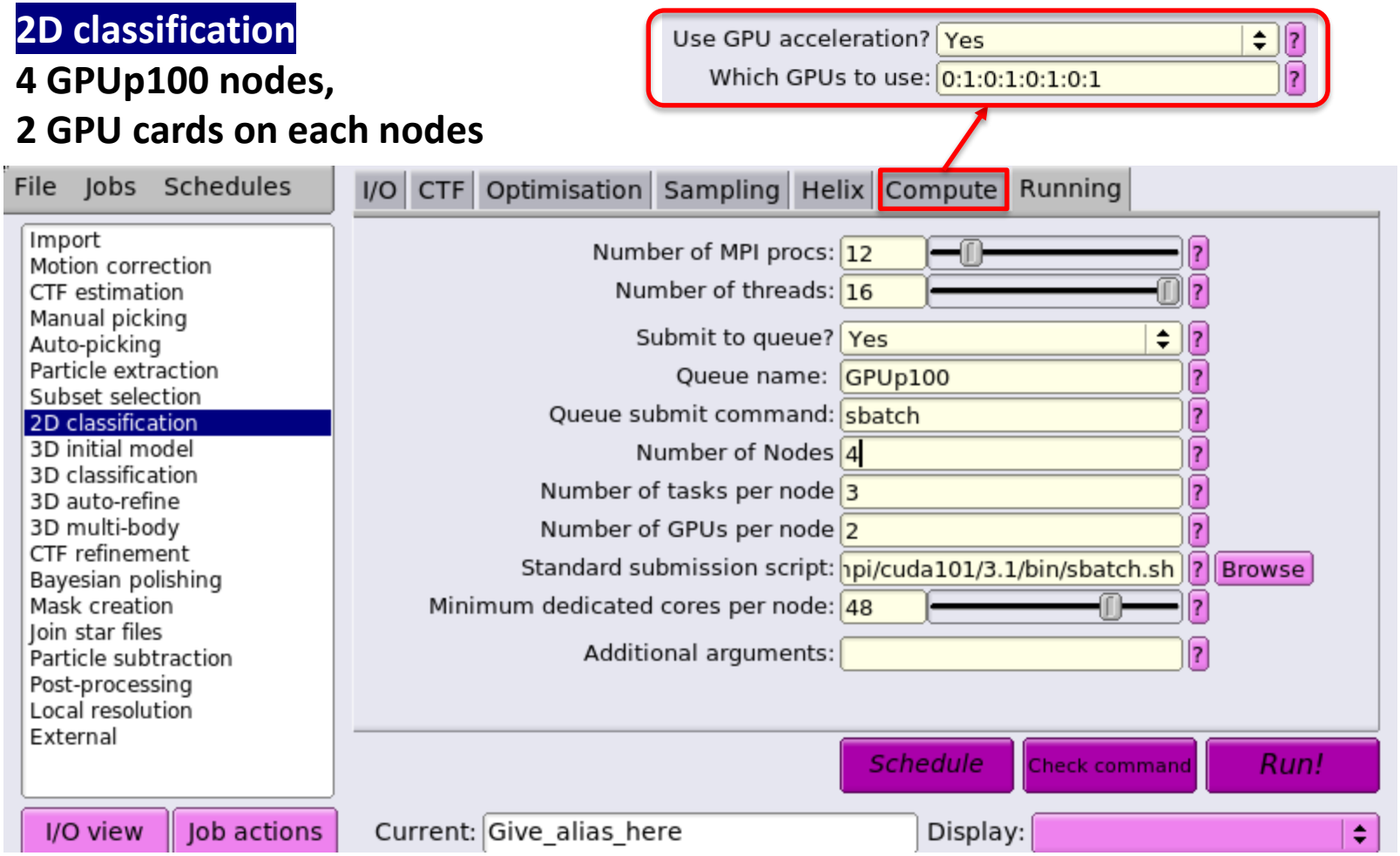


Examples of submitting RELION job to multiple nodes

2D classification

4 GPUp100 nodes,

2 GPU cards on each nodes



Examples of submitting RELION job to multiple nodes

RELION 3.1 Manual

Number of MPI procs 3

(Note that *when using the EM-algorithm*, 2D classification, 3D classification, 3D initial model and 3D auto-refine use one MPI process as a master, which does not do any calculations itself, but sends jobs to the other MPI processors. Therefore, we often run the EM-algorithm using a single worker MPI process on each of the available GPUs, so we specify 3 here to include the master and one workers on each of the two GPUs.)

The general rule for 2D classification, 3D classification, 3D initial model, and 3D auto-refine would be:

```
IF Num_of_GPU_per_Node == 1:
        Num_of_MPI = 3 * Num_of_Nodes;
IF Num_of_GPU_per_Node >1:
        Num_of_MPI = (Num_of_GPU_per_node + 1) * Num_of_Nodes;

Num_of_threads =  minimum_num_of_cores_per_Node * Num_of_Nodes / Num_of_MPI ;

Num_of_tasks_per_Node = Num_of_MPI / Num_of_Nodes;
```

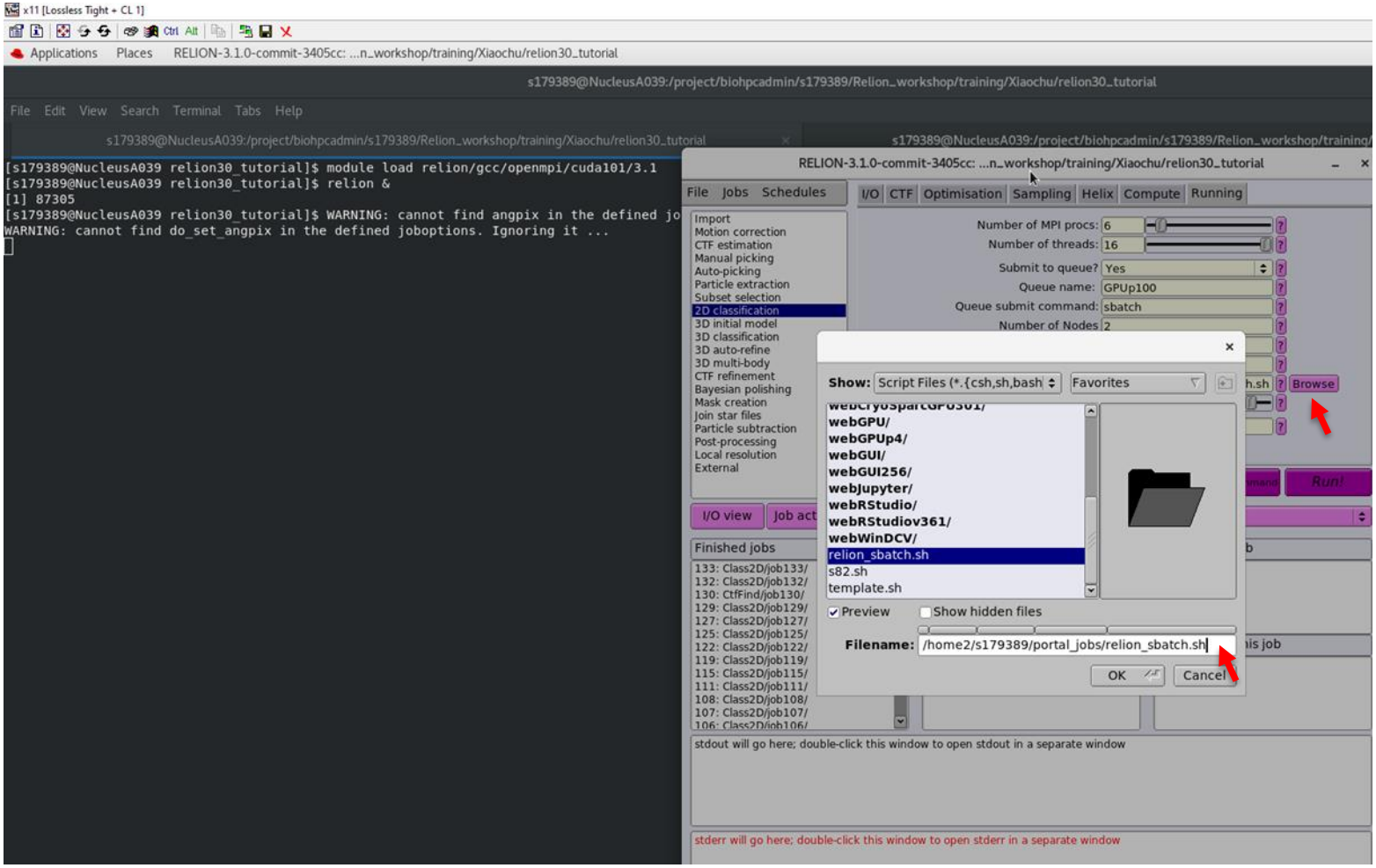
For other steps, eg, motion correction:

```
Num_of_MPI = Num_of_GPU_per_Node * Num_of_Nodes;
```

Standard RELION submit script

```
$ cat /cm/shared/apps/relion/gcc/openmpi/cuda101/3.1/bin/sbatch.sh
#!/bin/bash

#SBATCH --job-name RELIONJob
#SBATCH -p XXXqueueXXX          # partition (queue)
#SBATCH --nodes=XXXextra1XXX
#SBATCH --ntasks-per-node=XXXextra2XXX
##SBATCH --mem 250000           # Memory Requirement (MB)
##SBATCH -t 2-2:0:00
#SBATCH -o XXXoutfileXXX
#SBATCH -e XXXerrfileXXX
#SBATCH --gres=gpu:XXXextra3XXX

module load shared relion/gcc/openmpi/cuda101/3.1

mpiexec -n XXXmpinodesXXX XXXcommandXXX
```

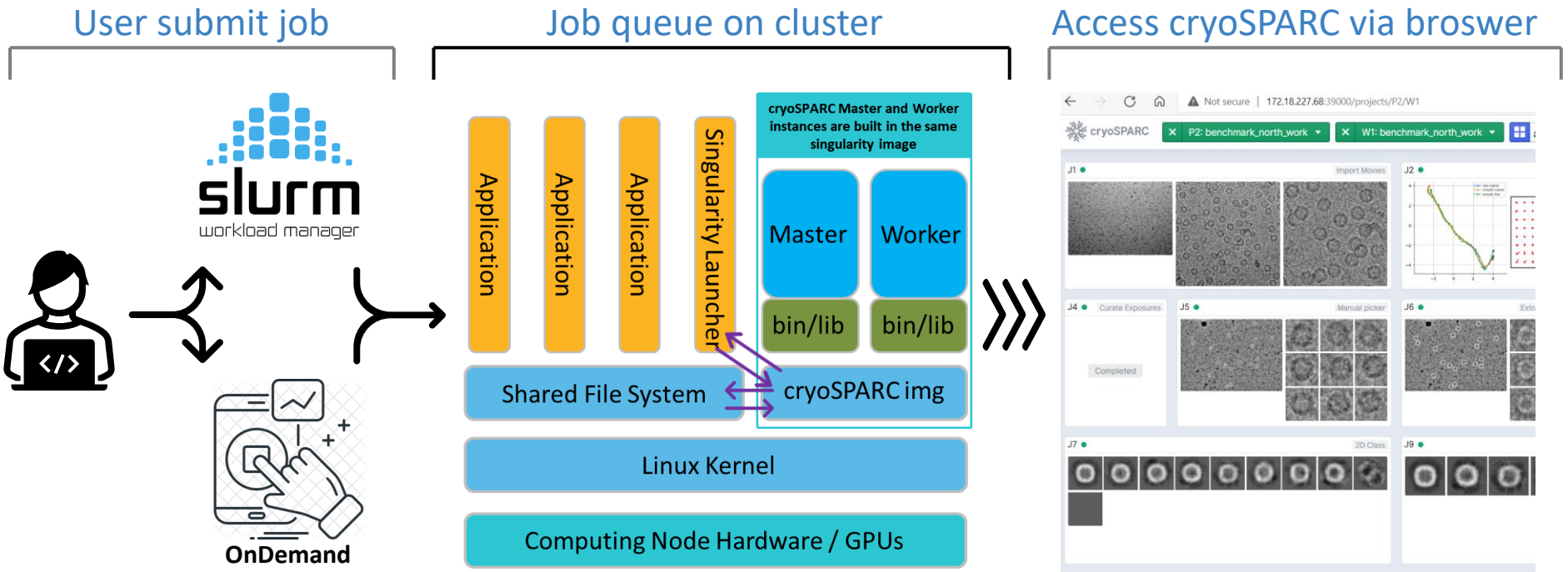
Create and use user defined submit script



Customize your RELION submit script

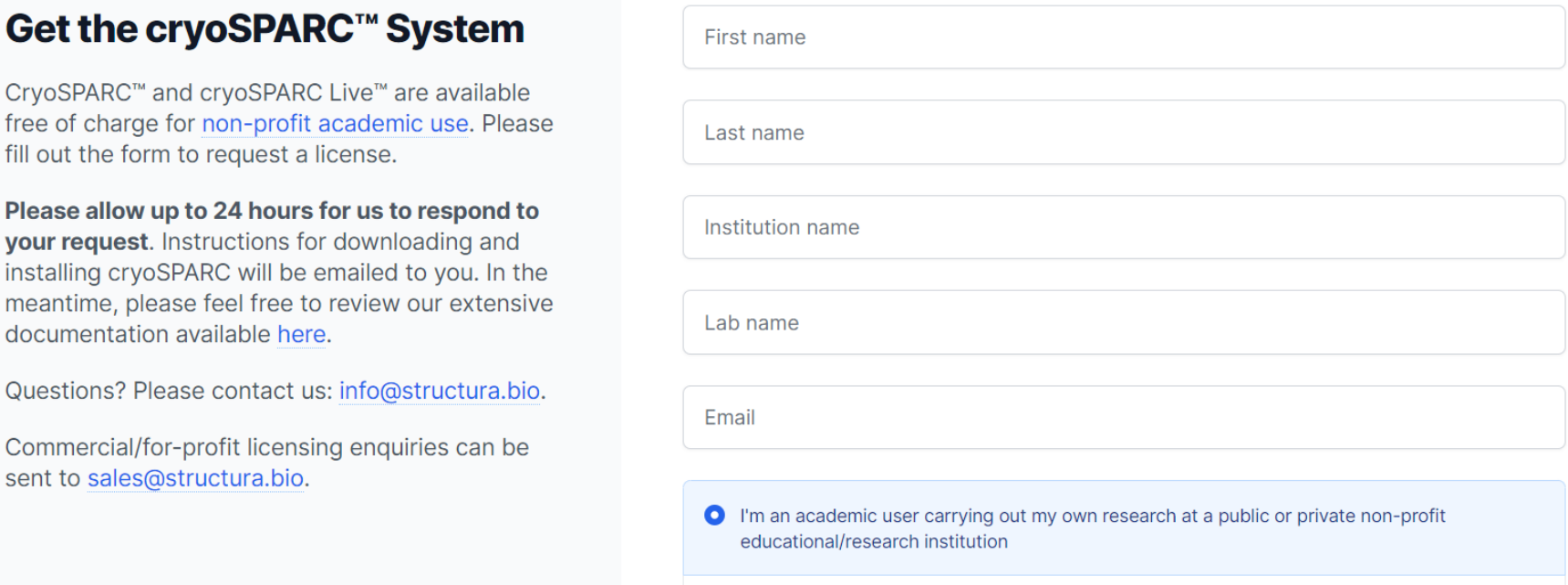
```
$ cat ~/portal_jobs/relion_sbatch.sh
#!/bin/bash

#SBATCH --job-name RELIONJob
#SBATCH -p XXXqueueXXX          # partition (queue)
#SBATCH --nodes=XXXextra1XXX
#SBATCH --ntasks-per-node=XXXextra2XXX
##SBATCH --mem 250000           # Memory Requirement (MB)
##SBATCH -t 1-2:0:00
#SBATCH -o XXXoutfileXXX
#SBATCH -e XXXerrfileXXX
#SBATCH --gres=gpu:XXXextra3XXX
#SBATCH --mail-type ALL
#SBATCH --mail-user xiaochu.lou@utsouthwestern.edu

module load shared relion/gcc/openmpi/cuda101/3.1
mpiexec -n XXXmpinodesXXX XXXcommandXXX
```

Containerization of cryoSPARC with Singularity



Get the cryoSPARC license

CryoSPARC™ and **cryoSPARC Live**™ are available free of charge for non-profit academic use. To obtain a License ID for cryoSPARC, go to cryosparc.com/download, fill out the form and submit it.



Get the cryoSPARC™ System

CryoSPARC™ and cryoSPARC Live™ are available free of charge for non-profit academic use. Please fill out the form to request a license.

Please allow up to 24 hours for us to respond to your request. Instructions for downloading and installing cryoSPARC will be emailed to you. In the meantime, please feel free to review our extensive documentation available here.

Questions? Please contact us: info@structura.bio.

Commercial/for-profit licensing enquiries can be sent to sales@structura.bio.

First name

Last name

Institution name

Lab name

Email

I'm an academic user carrying out my own research at a public or private non-profit educational/research institution

Export cryoSPARC license ID to user env

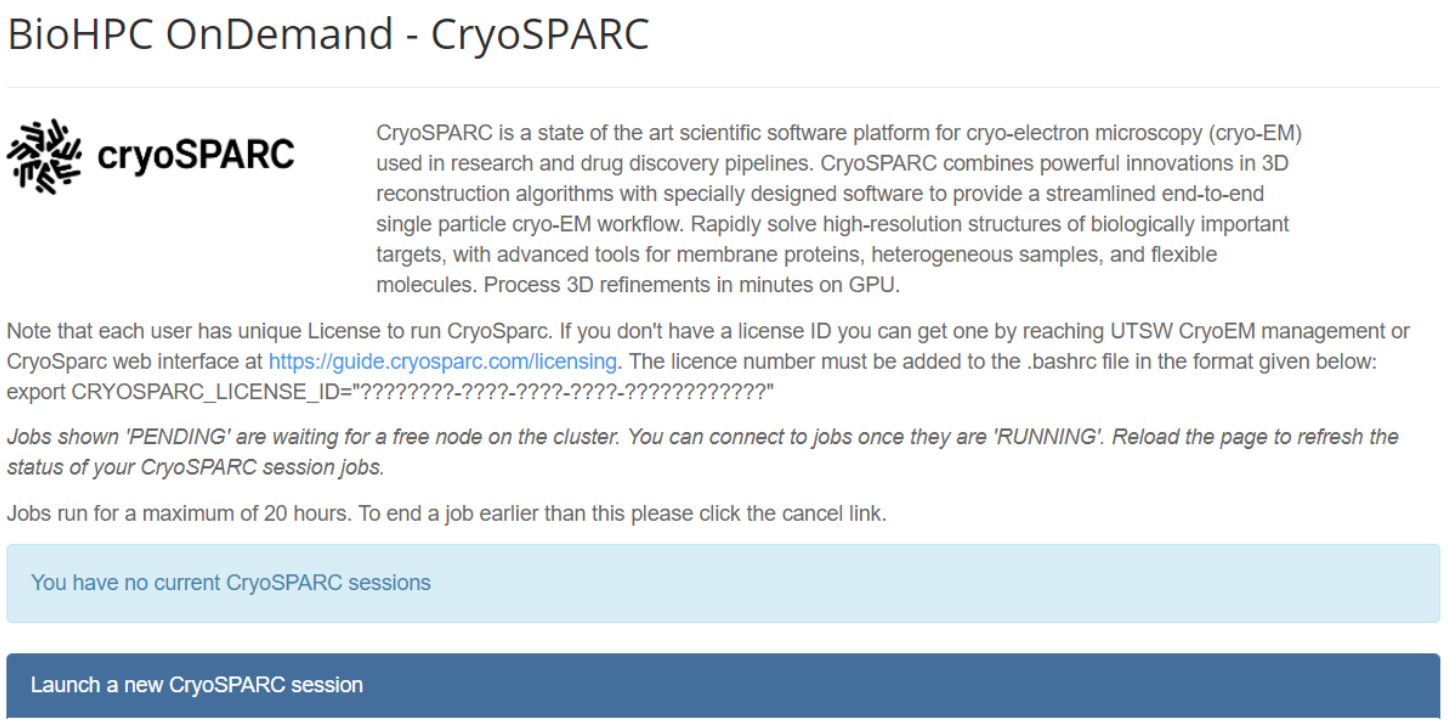
Step 1: Create a hidden file (.cryopwd) at user home2 directory, which is used to save the passwd for the cryoSPARC session. Note: Please use some random characters. DO NOT use important password of yours (eg, BioHPC account password)

```
[s179389@Nucleus006 ~]$ cat ~/.cryopwd
*********
```

Step 2: Add line "export CRYOSPARC_LICENSE_ID="????????-????-????-????-???????????" to export your cryoSPARC license ID to user .bashrc file.

```
[s179389@Nucleus006 ~]$ cat ~/.bashrc
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi

# User specific aliases and functions
module load slurm shared
export CRYOSPARC_LICENSE_ID="????????-????-????-????-???????????"
```

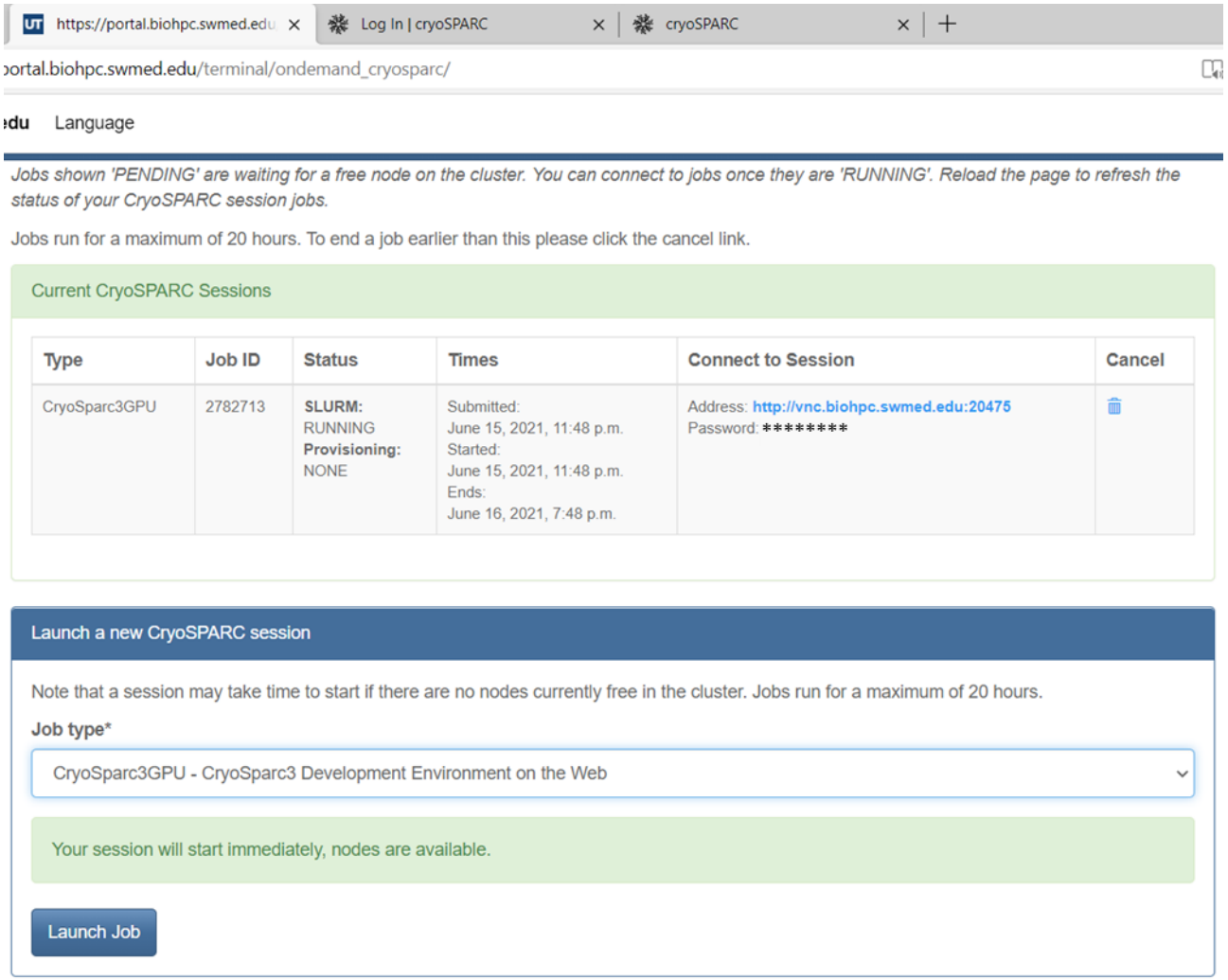
OnDemand cryoSPARC and cryoSPARC Live



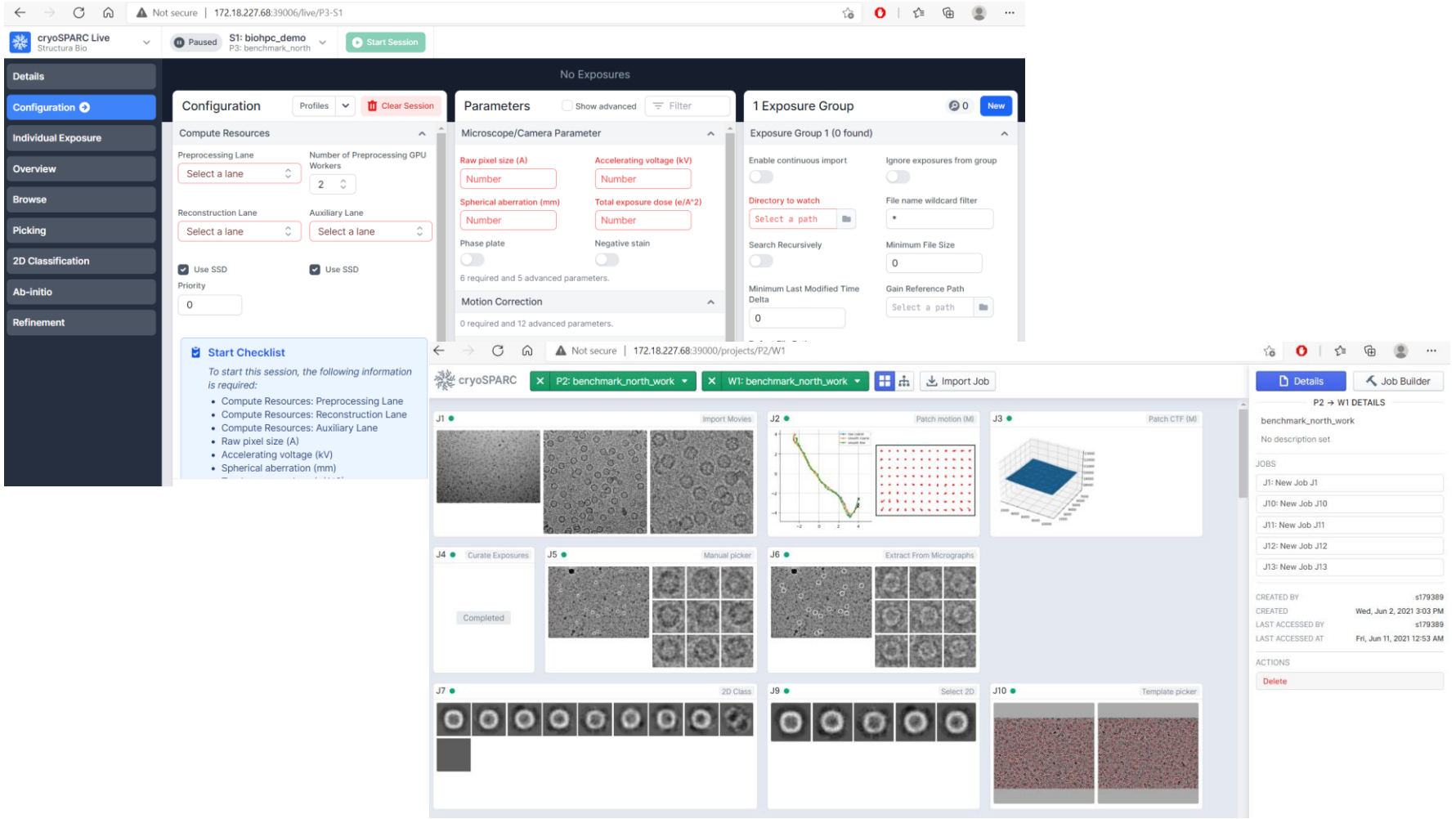
Guides about cryoSPARC usage:

1, BioHPC portal Guides page: [CryoEM resource on BioHPC (swmed.edu)]

OnDemand cryoSPARC and cryoSPARC Live



cryoSPARC and cryoSPARC Live



Submit slurm job to start cryoSPARC and cryoSPARC Live

```
$ cat ~/portal_jobs/cryosparc/cryosparc_sbatch_v100s.sh
#!/bin/bash
#SBATCH --job-name="Cryosparc3"
#SBATCH --partition=GPUv100s
#SBATCH --nodes=1
#SBATCH --gres=gpu:1  # Number of GPUs(per node)
#SBATCH --ntasks=1
#SBATCH --time=2-02:00:00
#SBATCH --output="logs.cryosprac3.%j.%N.txt"
#SBATCH --error=errors.cryosparc3.%j.%N.txt

module load cryosparc/3.3.2-singularity
export no_proxy="localhost"
export CUDA_VISIBLE_DEVICES=0
cryosparc start
tail -f ~/cryosparc-v3/run/command_core.log
```

Submit slurm job to start cryoSPARC and cryoSPARC Live

```
# Submit to start the job
[s179389@Nucleus005 ~]$ sbatch  ~/portal_jobs/cryosparc/cryosparc_sbatch_v100s.sh
Submitted batch job 2776433
# Check the cryoSPARC job initialization log
[s179389@Nucleus005 ~]$ cat ~/cryosparc-v3/cryosparc.log
……

 From other machines on the network, access cryoSPARC at
   http://Nucleus162.cm.cluster:39000
 and access cryoSPARC Live at
   http://Nucleus162.cm.cluster:39006

……
 Success starting cryosparc master!
……

Success starting cryosparc worker
Checking Licence validation !

……

FINISHED : Check ~/cryosparc-v3/run/command_core.log file for detail
```

Allocated node with cryoSPARC job running.
Connect to cryoSPARC web interface via:
172.18.224.162:39000 (39006: cryoSPARC Live)
The number is from Nucleus162

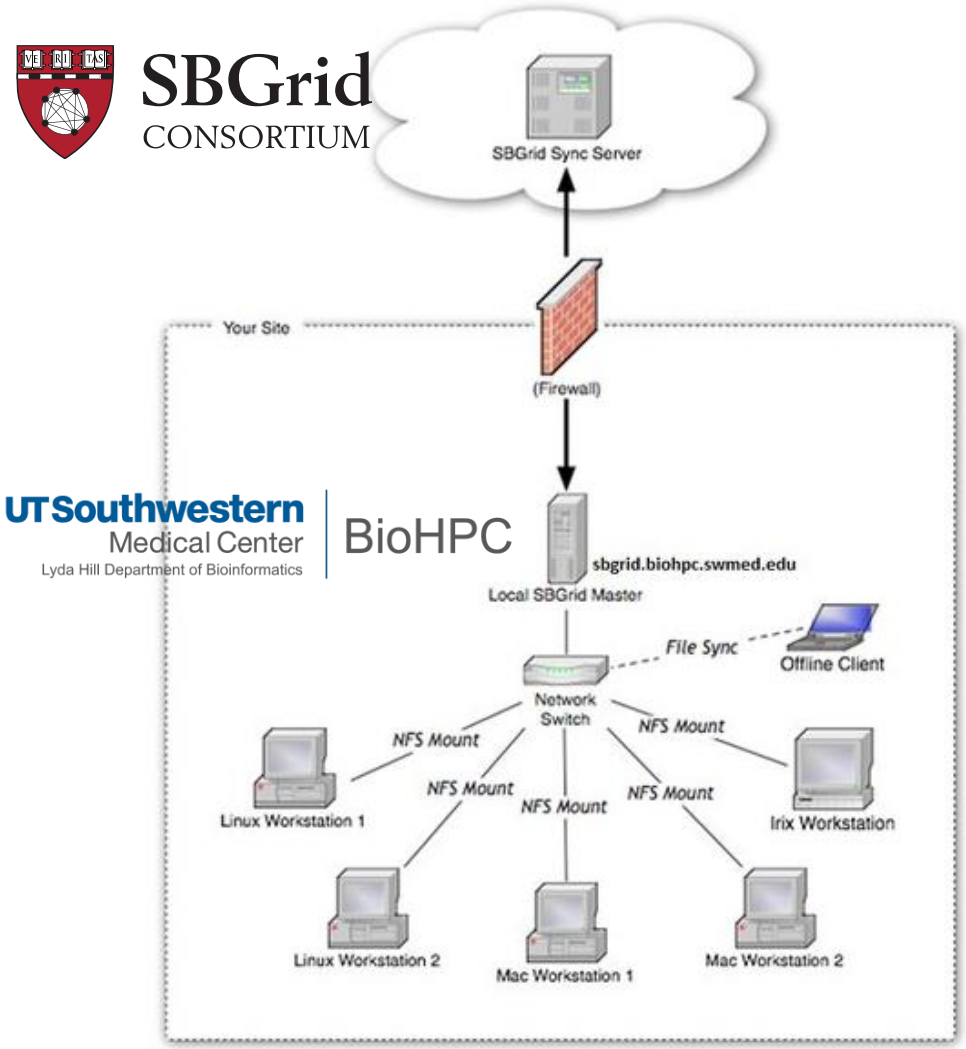
The other example, if the allocated node is NucleusC048; Connect to cryoSPARC web interface via:
172.18.227.48:39000 (39006: cryoSPARC Live)
The number is from NucleusC048

Submit slurm job to start cryoSPARC and cryoSPARC Live

```
# Submit to start the job
[s179389@Nucleus005 ~]$ sbatch  ~/portal_jobs/cryosparc/cryosparc_sbatch_v100s.sh
Submitted batch job 2776433

# Cancel the job after finished
[s179389@Nucleus005 ~]$ module load cryosparc/3.1.0-singularity
[s179389@Nucleus005 ~]$ squeue -u s179389
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           2776433     GPUp4 Cryospar  s179389  R       5:16      1 NucleusC014
[s179389@Nucleus005 ~]$ cryosparc_canceljob  2776433
user confirmed of job: 2776433 running on node: NucleusC014
CryoSPARC is running.
Stopping cryoSPARC
app: stopped
command_core: stopped
command_rtp: stopped
command_vis: stopped
liveapp: stopped
webapp: stopped
database: stopped
Shut down
```

Note: before first time use:
Create a file named ~/.cryopwd and write your Cryosparc password to the first line without any space.

Initializing and Use SBGrid on BioHPC



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****
****

Information about joining SBGRID can be obtained from the SBGRID consortium via: https://sbgrid.org/join/

Guides about SBGrid usage:

1, BioHPC portal Guides page: SBGrid on BioHPC (swmed.edu)

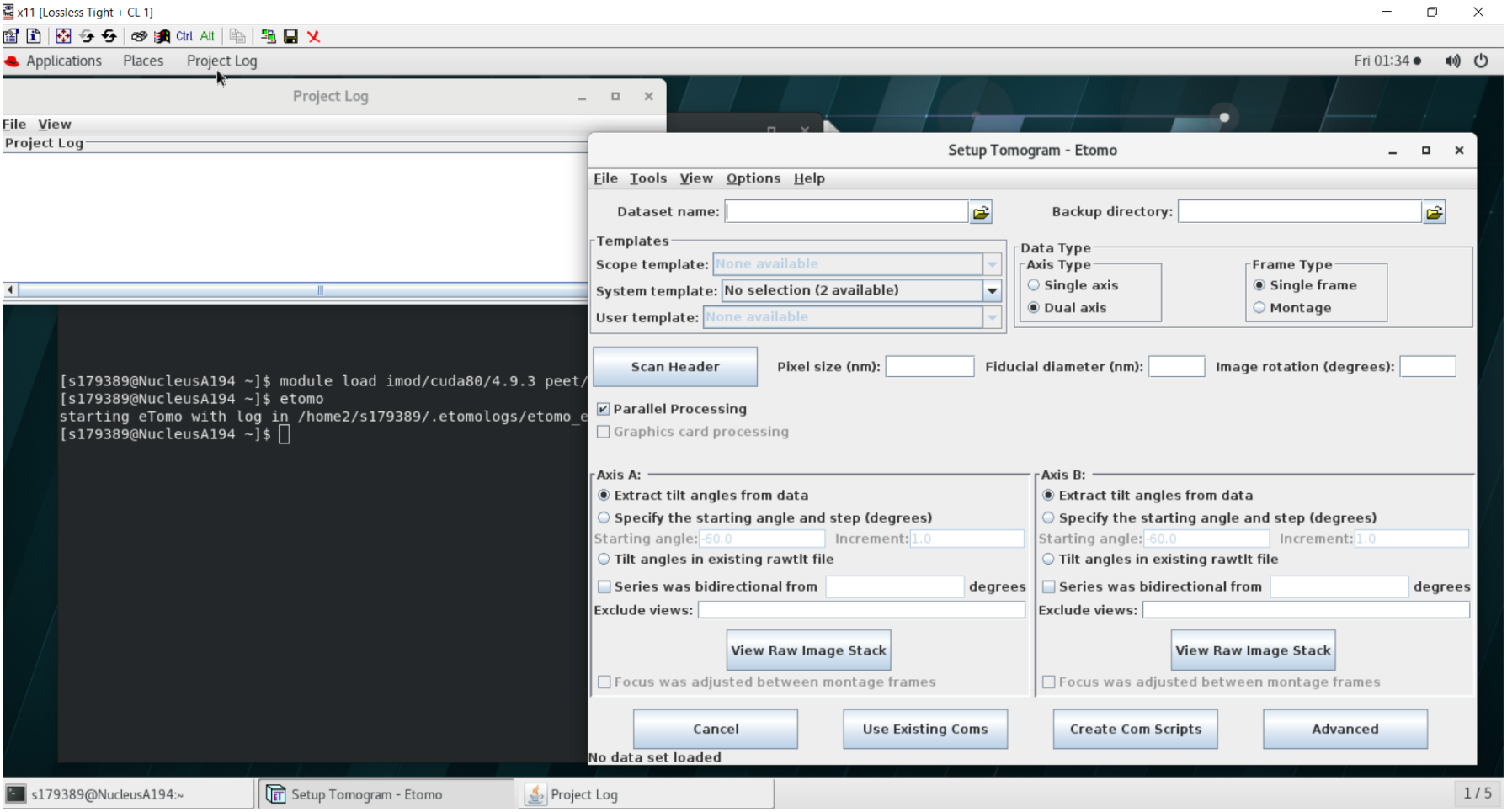
Initializing and Use SBGrid on BioHPC

```
[s179389@Nucleus005 ~]$ cat ~/.bashrc
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi

# User specific aliases and functions
module load slurm/16.05.8 shared

alias data='cd /project/biohpcadmin/s179389'

#sbgrid initializing
. /programs/sbgrid.shrc
```

Initializing and Use SBGrid on BioHPC

```
********************************************************************************
                  Software Support by SBGrid (www.sbgrid.org)
********************************************************************************
 Your use of the applications contained in the /programs  directory constitutes
 acceptance of  the terms of the SBGrid License Agreement included  in the file
 /programs/share/LICENSE.  The applications  distributed by SBGrid are licensed
 exclusively to member laboratories of the SBGrid Consortium.
             Run sbgrid-accept-license to remove the above message.
********************************************************************************
 SBGrid was developed with support from its members, Harvard Medical School,
 HHMI, and NSF. If use of SBGrid compiled software was an important element
 in your publication, please include the following reference in your work:

 Software used in the project was installed and configured by SBGrid.
 cite: eLife 2013;2:e01456, Collaboration gets the most out of software.
********************************************************************************
 SBGrid installation last updated: 2021-03-05 (Update available)
 Please submit bug reports and help requests to:       <bugs@sbgrid.org>  or
                                                       <http://sbgrid.org/bugs>
           For additional information visit https://sbgrid.org/wiki
********************************************************************************
                              SBGrid Announcements
 - There are known issues with MacOS 11.0 “Big Sur” and some SBGrid
   applications. We recommend not upgrading Apple computers to 11.0
   until these issues can be addressed.
     see https://sbgrid.org/wiki/big_sur for more info.
********************************************************************************
[s179389@Nucleus006 ~]$ which relion
/programs/x86_64-linux/system/sbgrid_bin/relion
[s179389@Nucleus006 ~]$ module load relion/gcc/openmpi/cuda101/3.1
[s179389@Nucleus006 ~]$ which relion
/cm/shared/apps/relion/gcc/openmpi/cuda101/3.1/bin/relion
```

Use IMOD and PEET on BioHPC



UT Southwestern Medical Center
Lyda Hill Department of Bioinformatics

BioHPC

CryoSPARC/Relion Workshop (SBL/BioHPC)

Questions? Comments?

Email: biohpc-help@utsouthwestern.edu

Thanks!

UT Southwestern Medical Center

Lyda Hill Department of Bioinformatics

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