Neuroimaging on the Shared Computing Cluster (SCC)

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Resources

- Tutorial Slides will be made available:
  - https://www.bu.edu/tech/support/research/training-consulting/access-training-materials/

- Questions, Problems, Need Help?
  - help@scc.bu.edu
  - mhorn@bu.edu

Topics

- Get On the SCC
- What/Where/How the SCC?
- OnDemand
- Unix
- Wrangling Imaging Data
- XNAT
- Using the Batch System
- Useful Tools

Topics

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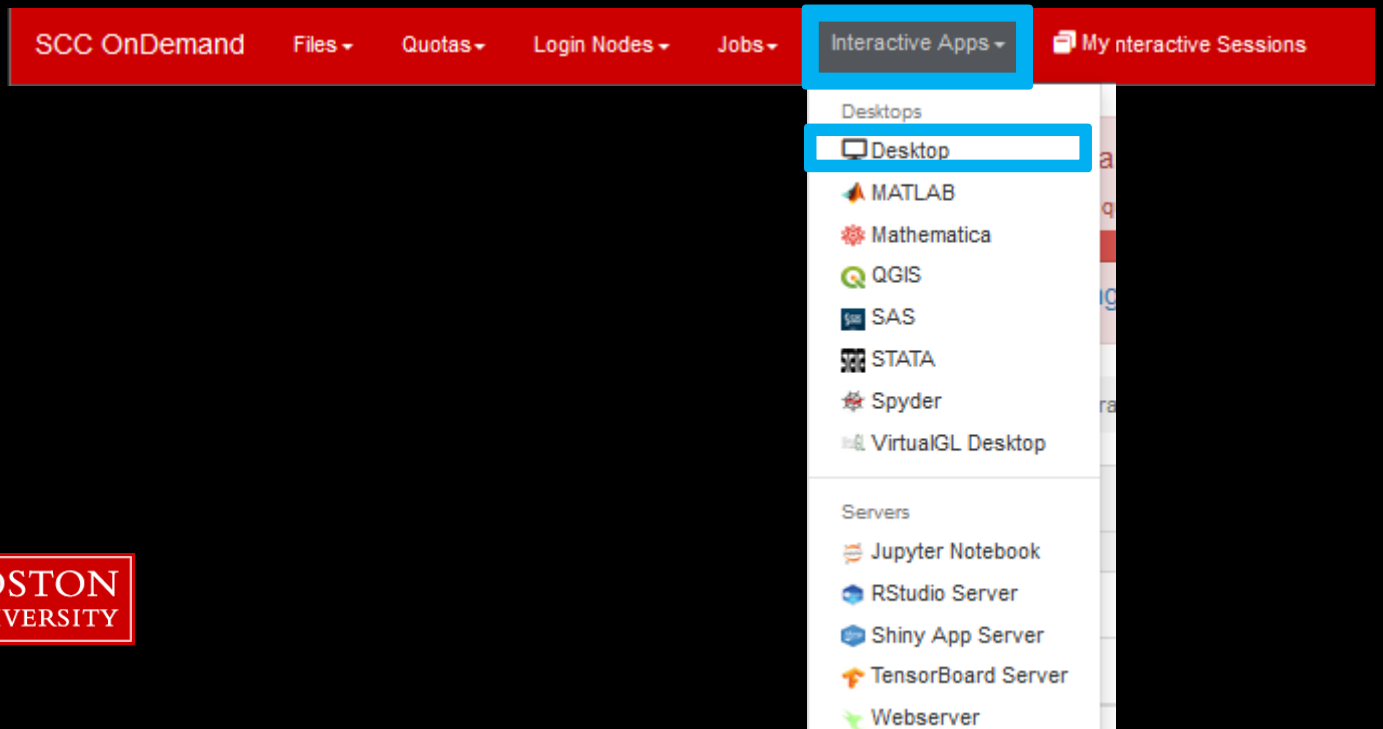
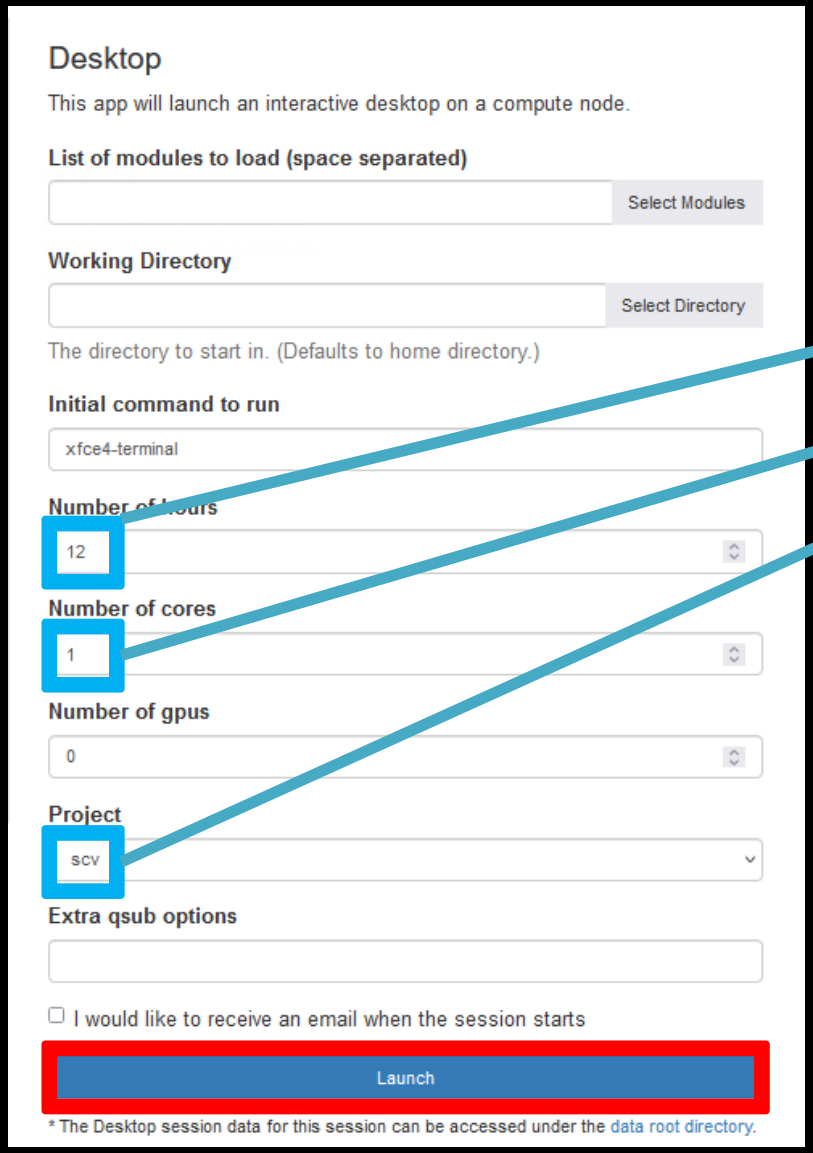
Connect to OnDemand

1. Go to: scc-ondemand-tutorial.bu.edu
2. Username: **tuta#** [random # between 30-99]
3. Password: **Yardbirds#**
4. Click: Interactive Apps
5. Click: Desktop



Connect to OnDemand



3 hours

1 core

project-ID

click launch!

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Topics

- Get On the SCC
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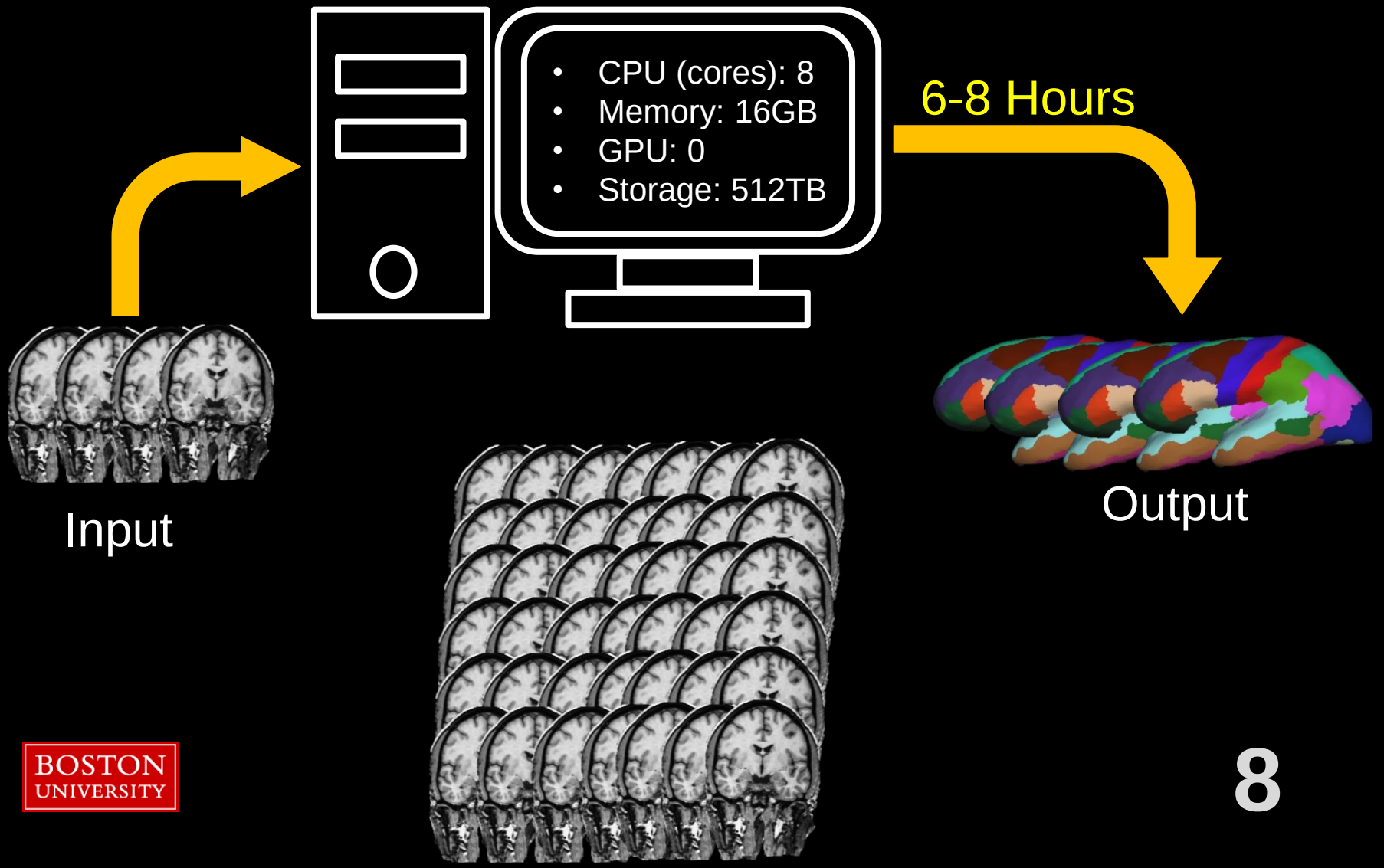
- Useful Tools

What is the SCC?



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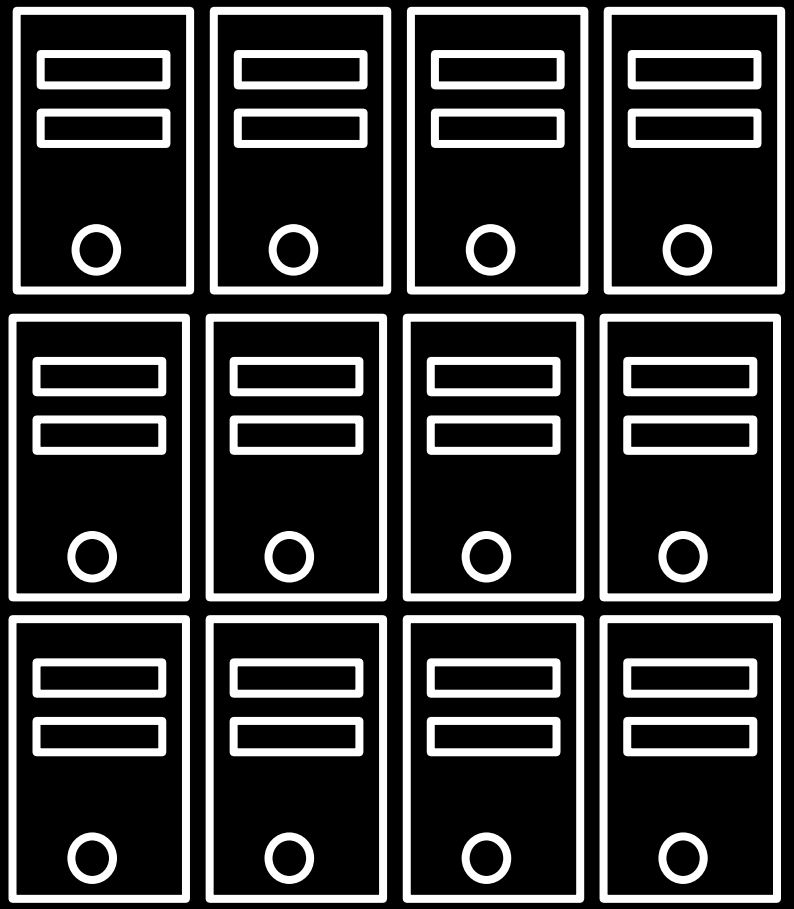
What is the SCC?

- > 900 Computers (nodes)
- > 25,000 CPUs (cores)
- > 100 GPUs
- > 9 PB (storage)



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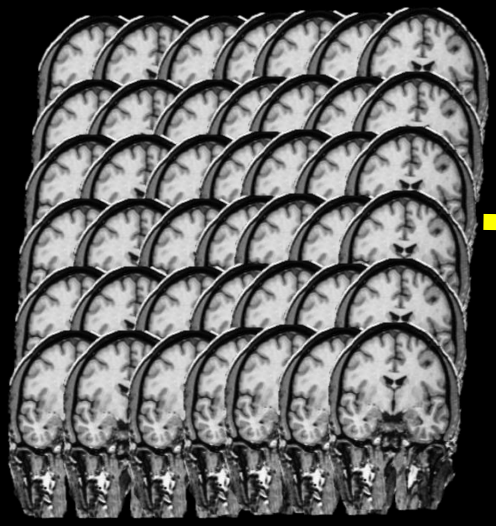
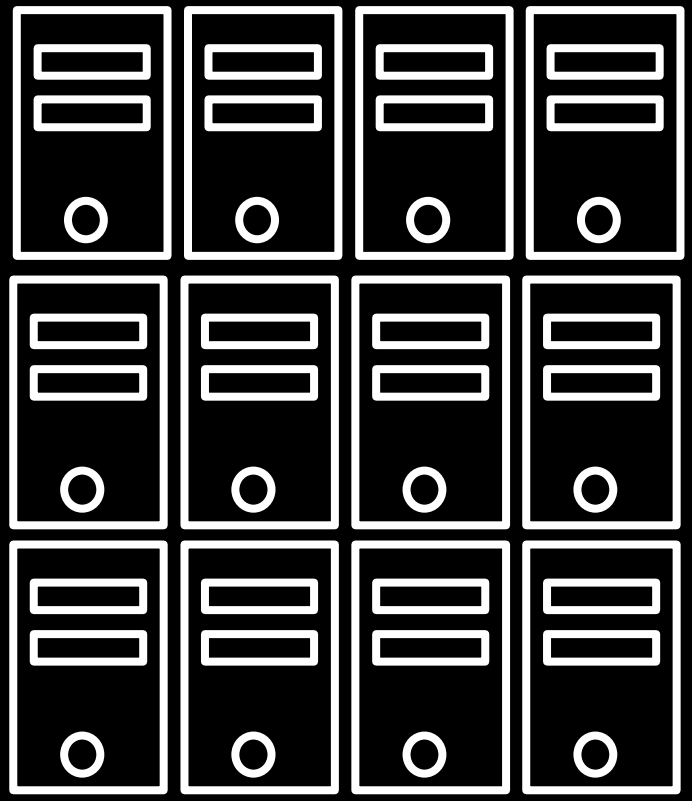
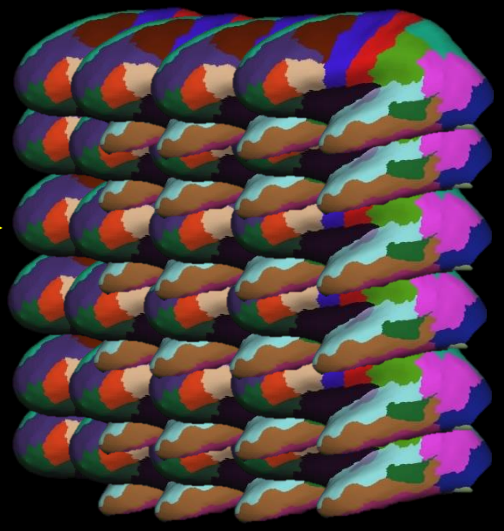
What is the SCC?

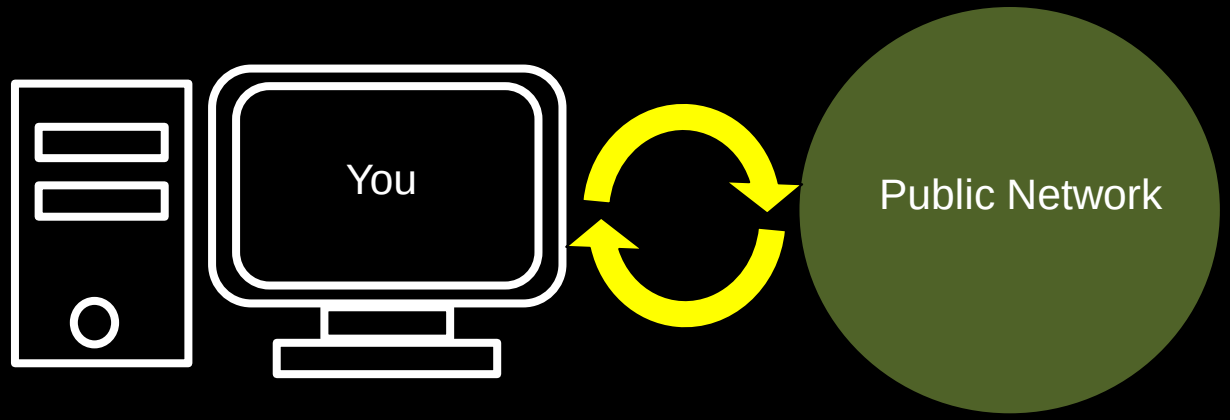




6-8 Hours



How to Connect to the SCC?



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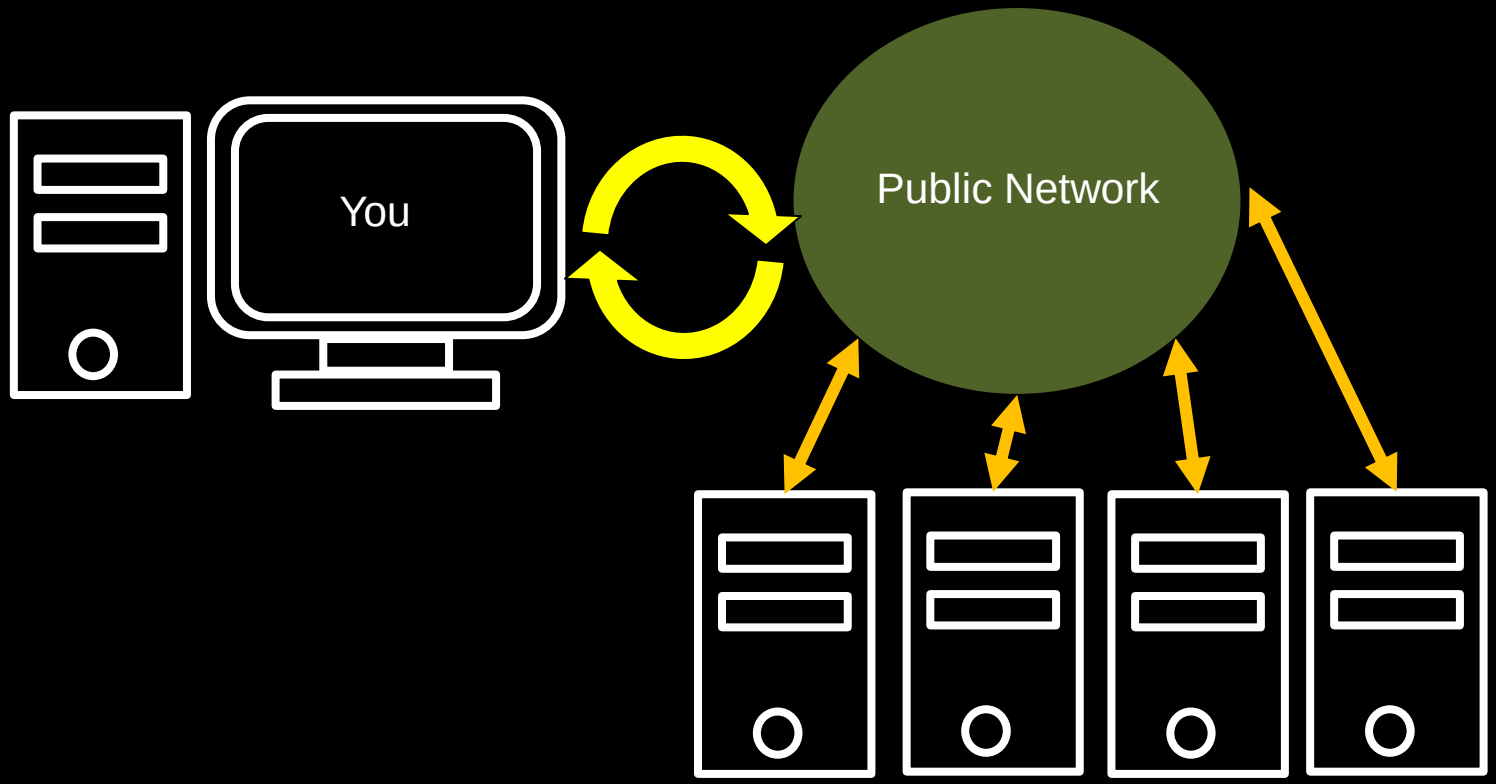
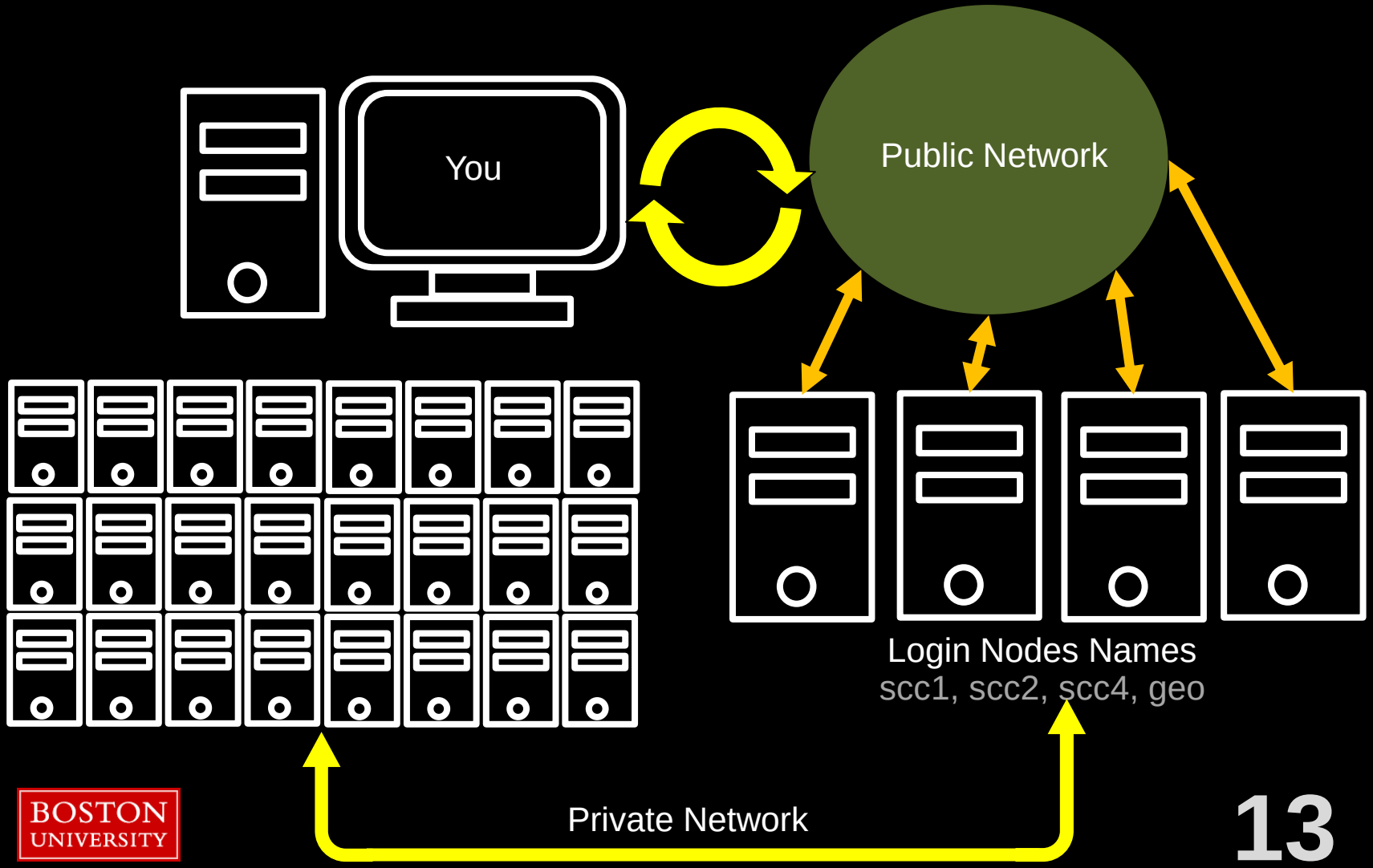


How to Connect to the SCC?



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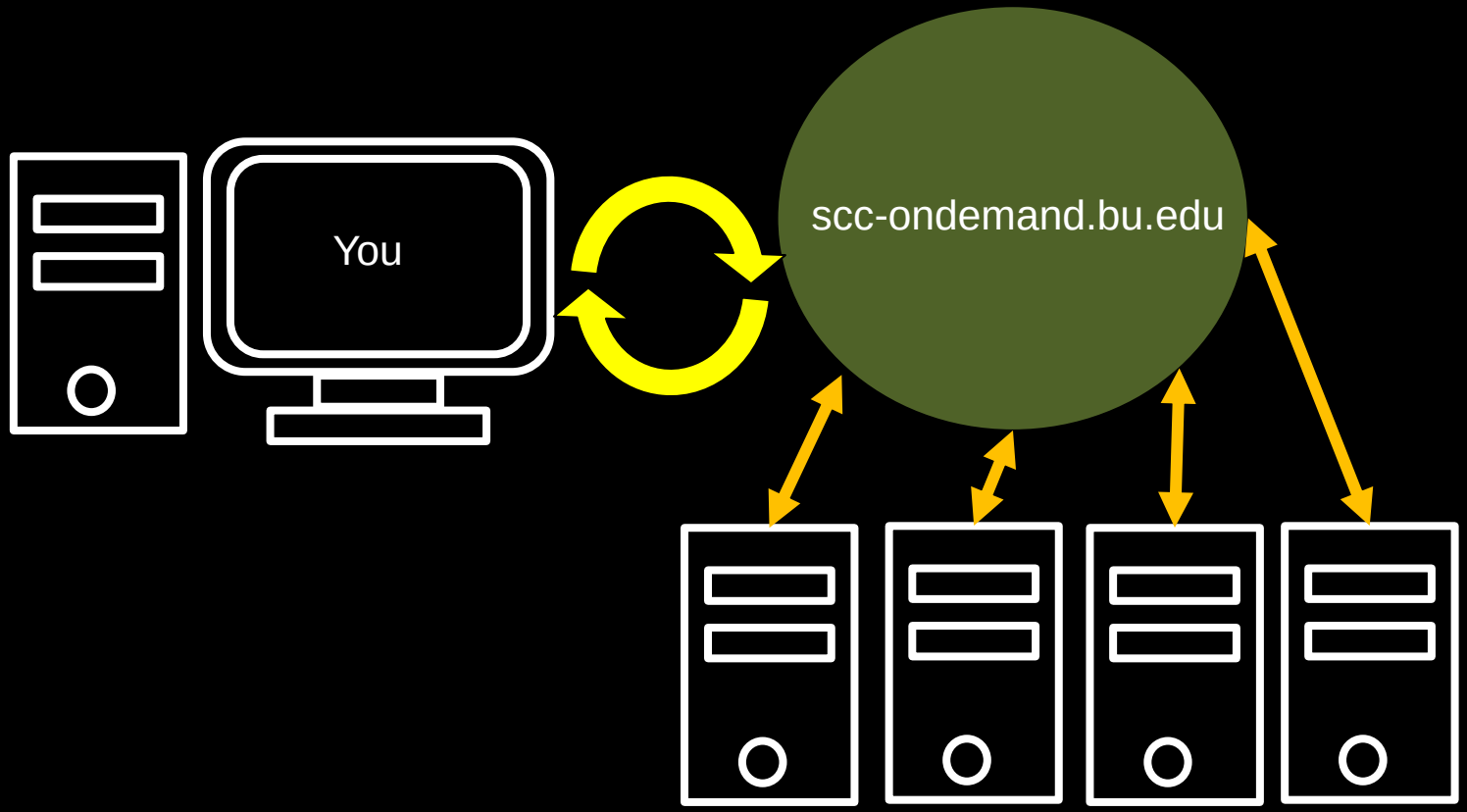

Getting an SCC Account?

- Using tutorial accounts today. These should not be used after today.
- All users of the SCC must be on a Research Project headed up by a full-time BU Faculty member.
- Exception: Some classes may have an academic project which you can be added to for the semester

- http://www.bu.edu/tech/support/research/account-management/

Questions so Far?

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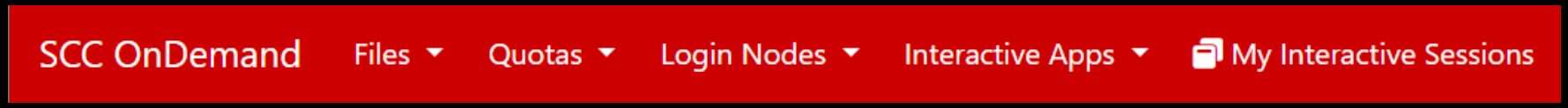
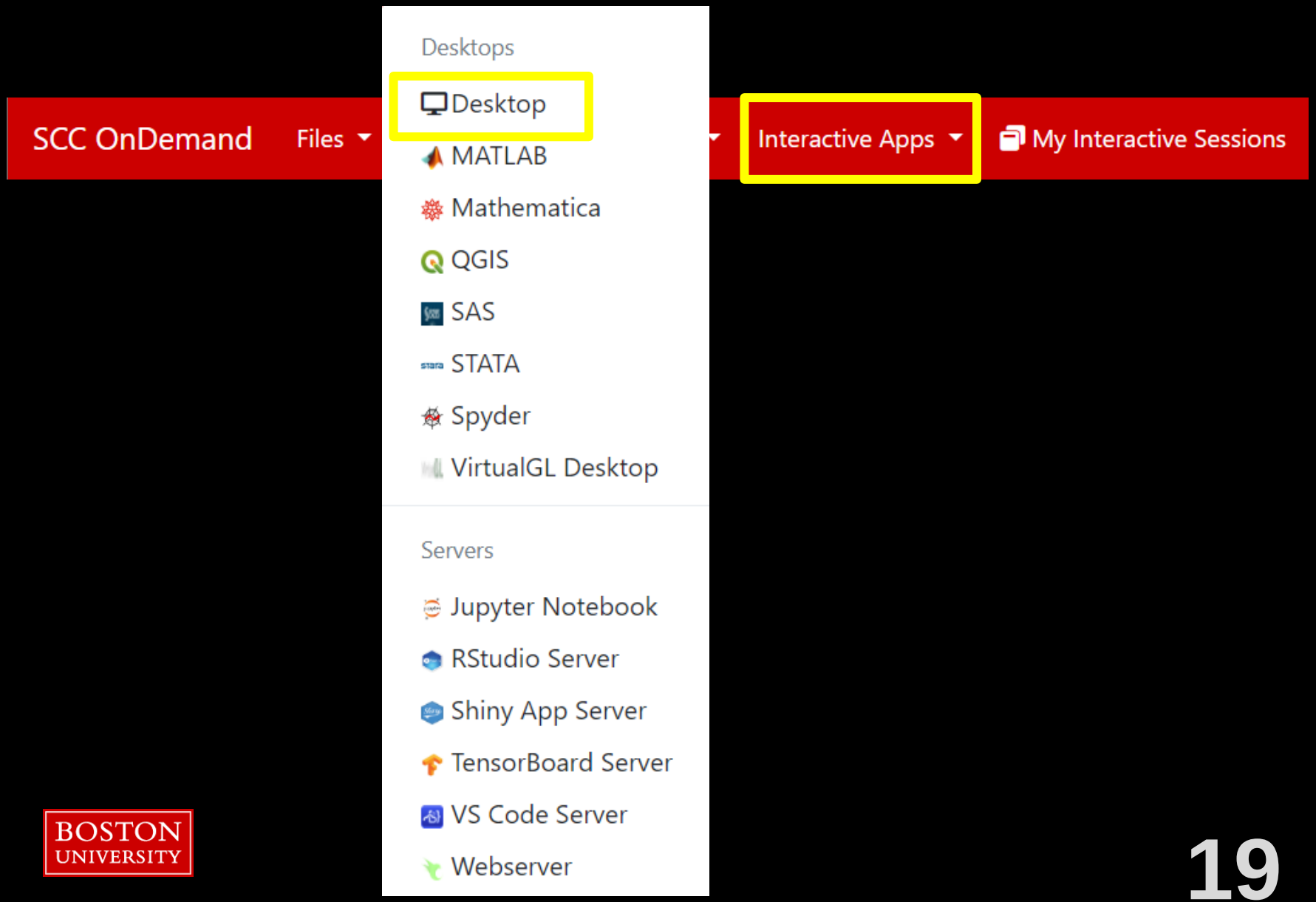
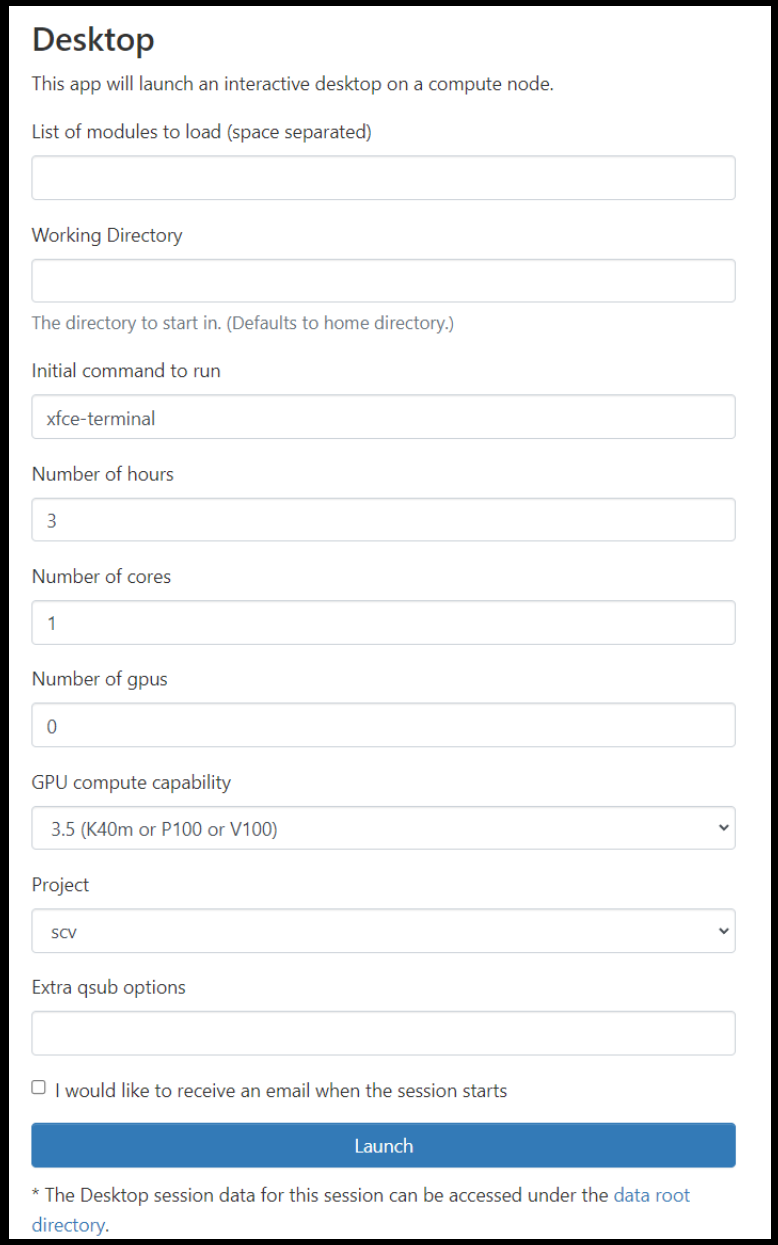
OnDemand


SCC OnDemand
Files
Quotas
Login Nodes
Interactive Apps
My Interactive Sessions

OnDemand


SCC OnDemand
Files
Interactive Apps
My Interactive Sessions
Desktops
Desktop
MATLAB
Mathematica
QGIS
SAS
STATA
Spyder
VirtualGL Desktop
Servers
Jupyter Notebook
RStudio Server
Shiny App Server
TensorBoard Server
VS Code Server
Webserver

OnDemand



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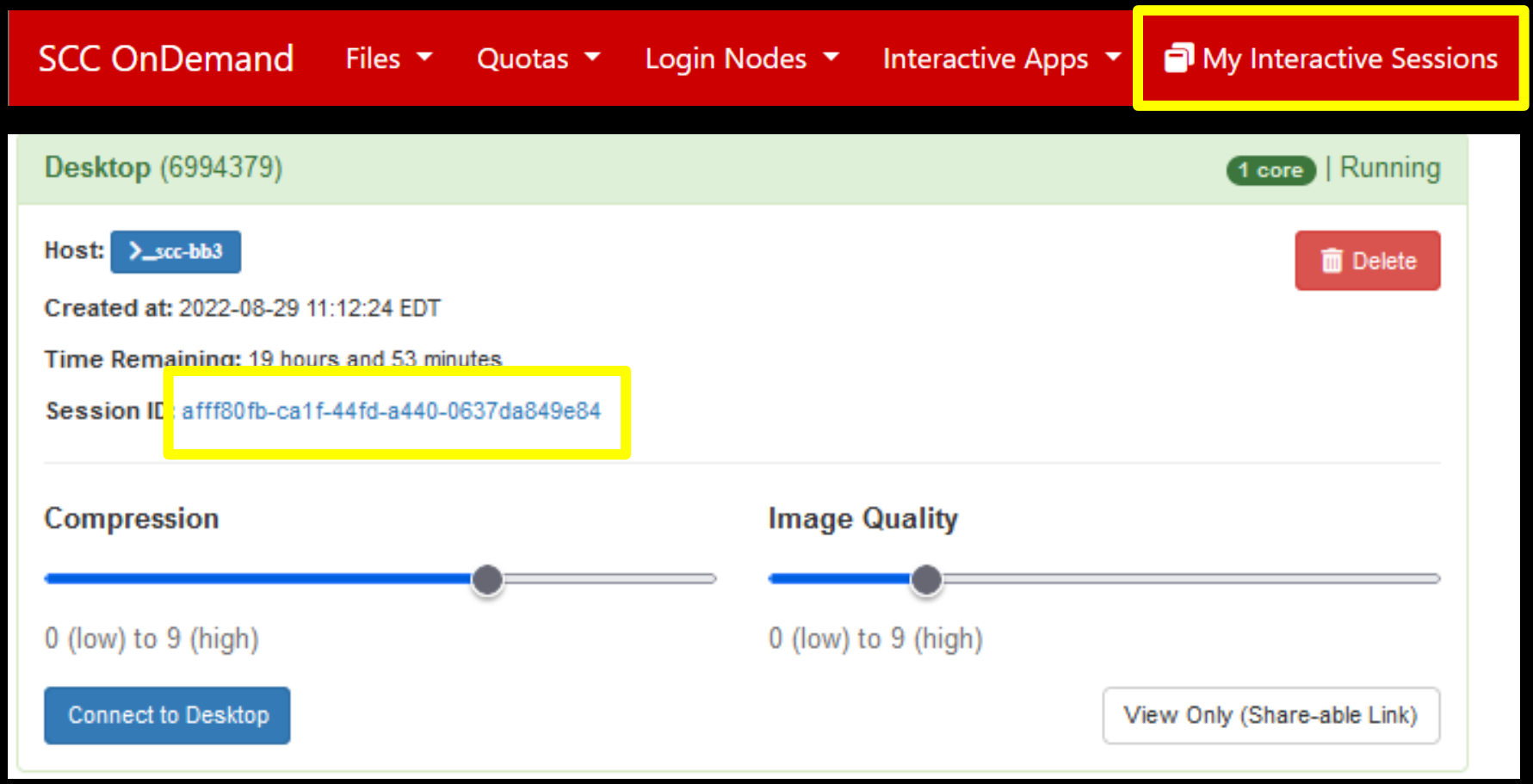
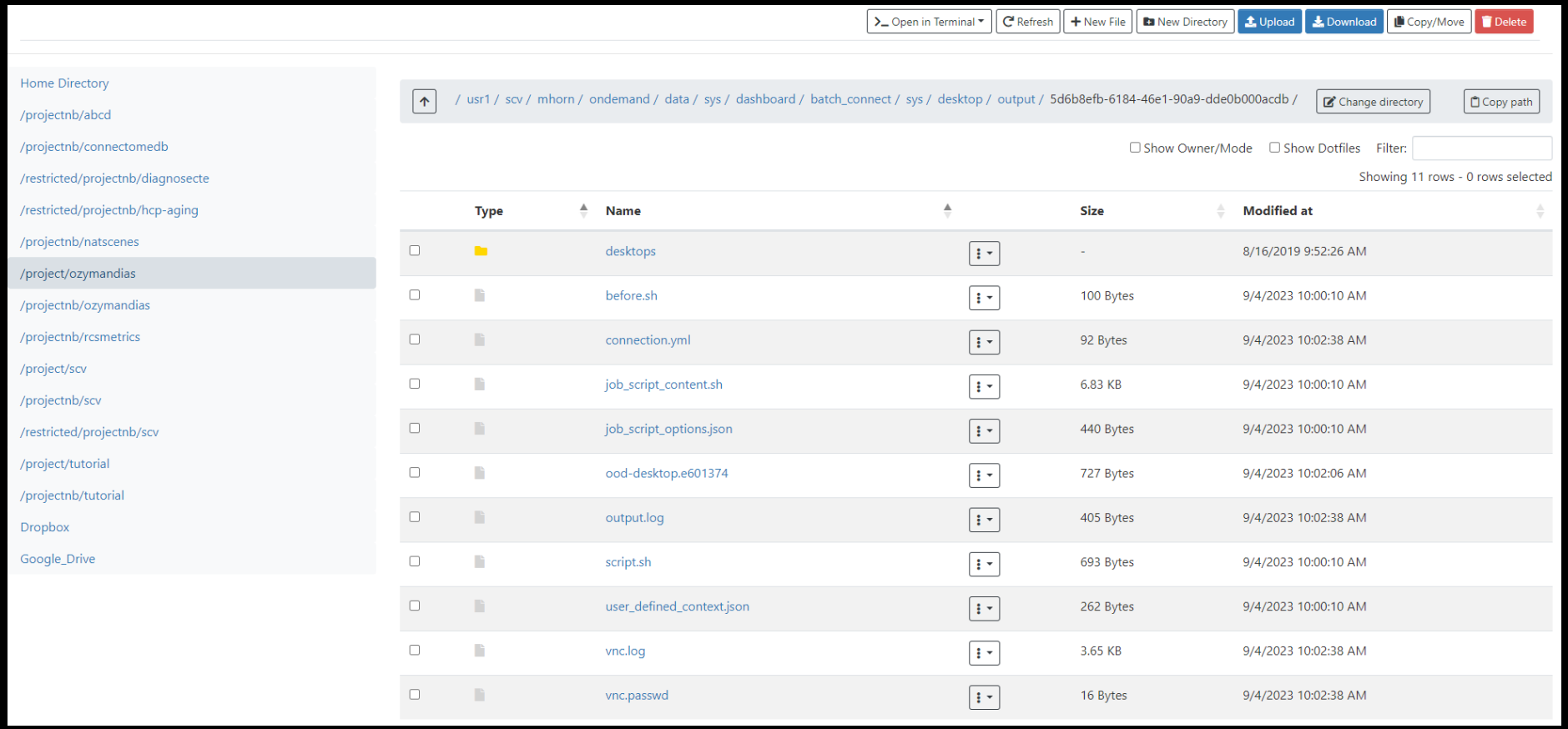
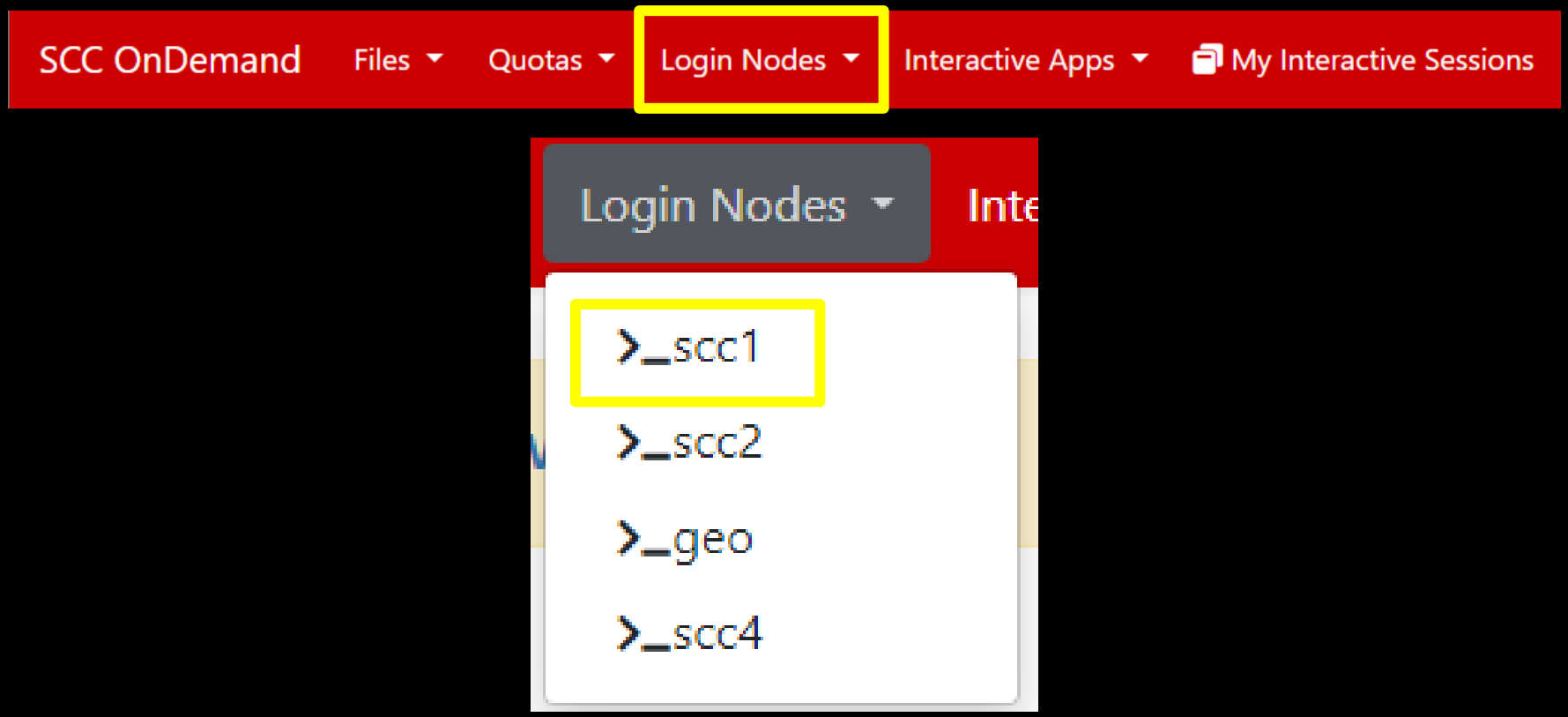
OnDemand


SCC OnDemand
Files
Quotas
Login Nodes
Interactive Apps
My Interactive Sessions
Desktop (6994379)
1 core | Running
Host: >_scc-bb3
Delete
Created at: 2022-08-29 11:12:24 EDT
Time Remaining: 19 hours and 53 minutes
Session ID: afff80fb-ca1f-44fd-a440-0637da849e84
Compression
Image Quality
0 (low) to 9 (high)
0 (low) to 9 (high)
Connect to Desktop
View Only (Share-able Link)

OnDemand


Open in Terminal
Refresh
New File
New Directory
Upload
Download
Copy/Move
Delete
Home Directory
/projectnb/abcd
/projectnb/connectomedb
/restricted/projectnb/diagnosecte
/restricted/projectnb/hcp-aging
/projectnb/natscenes
/project/ozymandias
/projectnb/ozymandias
/projectnb/rcsmetrics
/project/scv
/projectnb/scv
/restricted/projectnb/scv
/project/tutorial
/projectnb/tutorial
Dropbox
Google_Drive
/ usr1 / scv / mhorn / ondemand / data / sys / dashboard / batch_connect / sys / desktop / output / 5d6b8efb-6184-46e1-90a9-dde0b000acdb /
Change directory
Copy path
Show Owner/Mode
Show Dotfiles
Filter:
Showing 11 rows - 0 rows selected
Type
Name
Size
Modified at
desktops - 8/16/2019 9:52:26 AM
before.sh 100 Bytes 9/4/2023 10:00:10 AM
connection.yml 92 Bytes 9/4/2023 10:02:38 AM
job_script_content.sh 6.83 KB 9/4/2023 10:00:10 AM
job_script_options.json 440 Bytes 9/4/2023 10:00:10 AM
ood-desktop.e601374 727 Bytes 9/4/2023 10:02:06 AM
output.log 405 Bytes 9/4/2023 10:02:38 AM
script.sh 693 Bytes 9/4/2023 10:00:10 AM
user_defined_context.json 262 Bytes 9/4/2023 10:00:10 AM
vnc.log 3.65 KB 9/4/2023 10:02:38 AM
vnc.passwd 16 Bytes 9/4/2023 10:02:38 AM

OnDemand – Login Nodes



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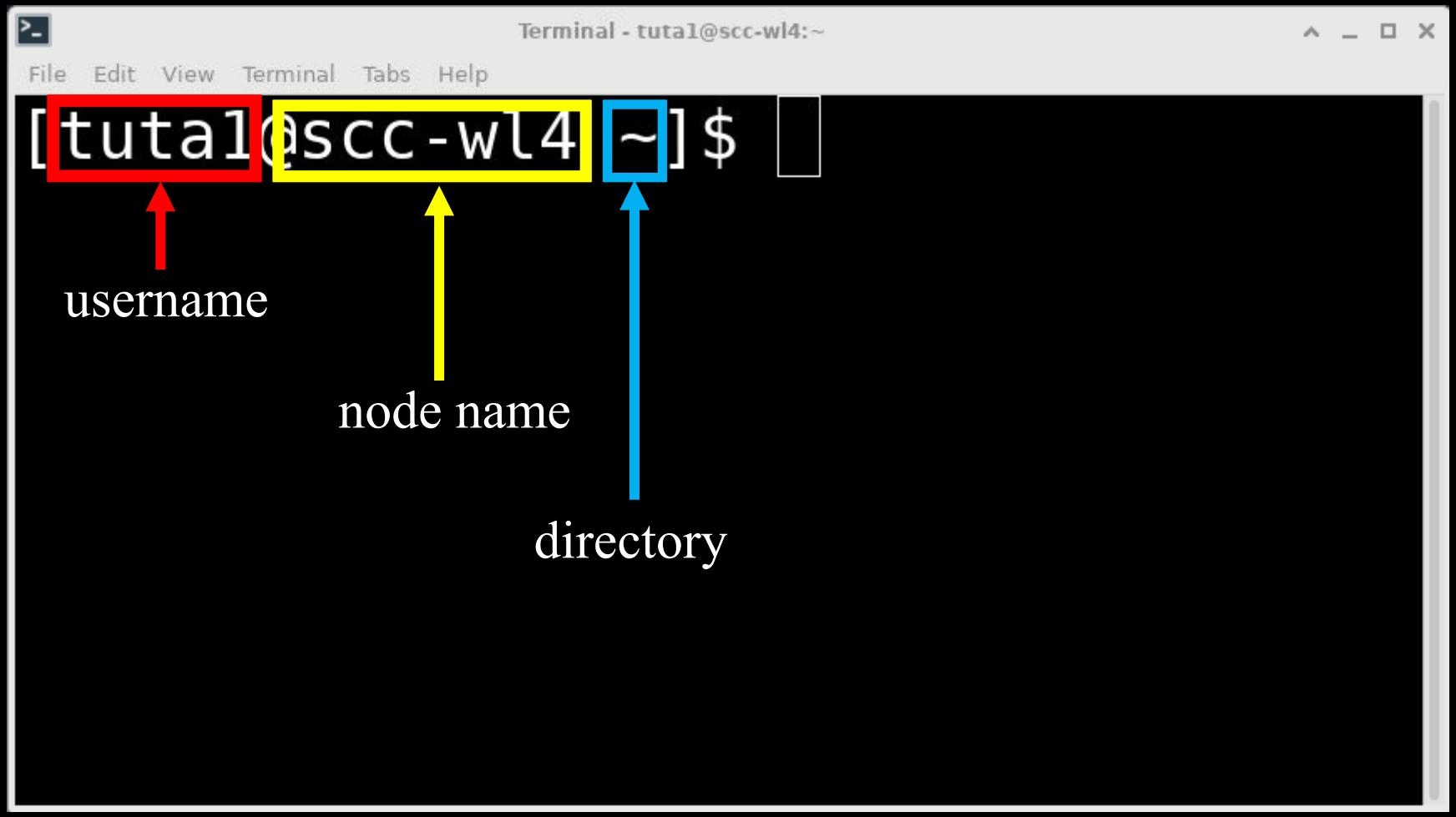
Unix



~ is shorthand for home directory

Unix

```
[tuta1@scc-v01 ~]$ groups
tutorial
```

The first group listed is your default project

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Unix

```
[tuta1@scc-v01 ~]$ pwd
/usr4/tutorial/tuta1
```

Shows the directory you are in, with the full path

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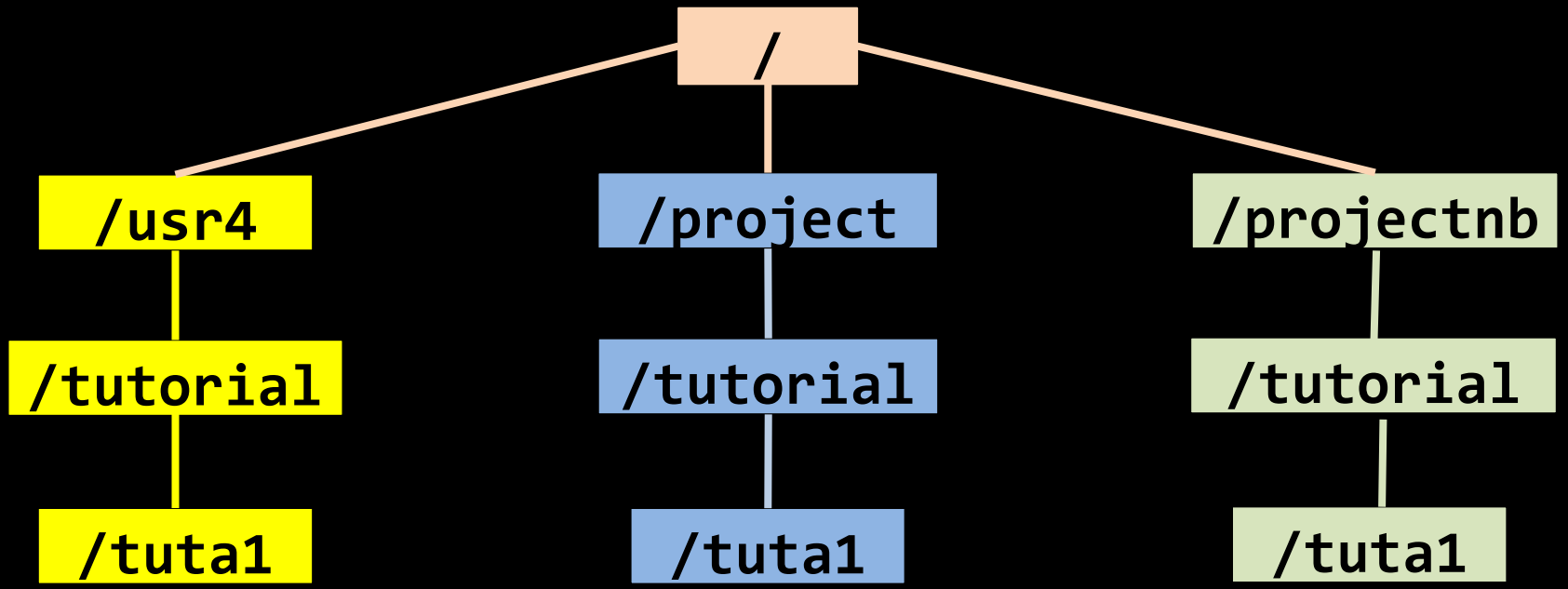
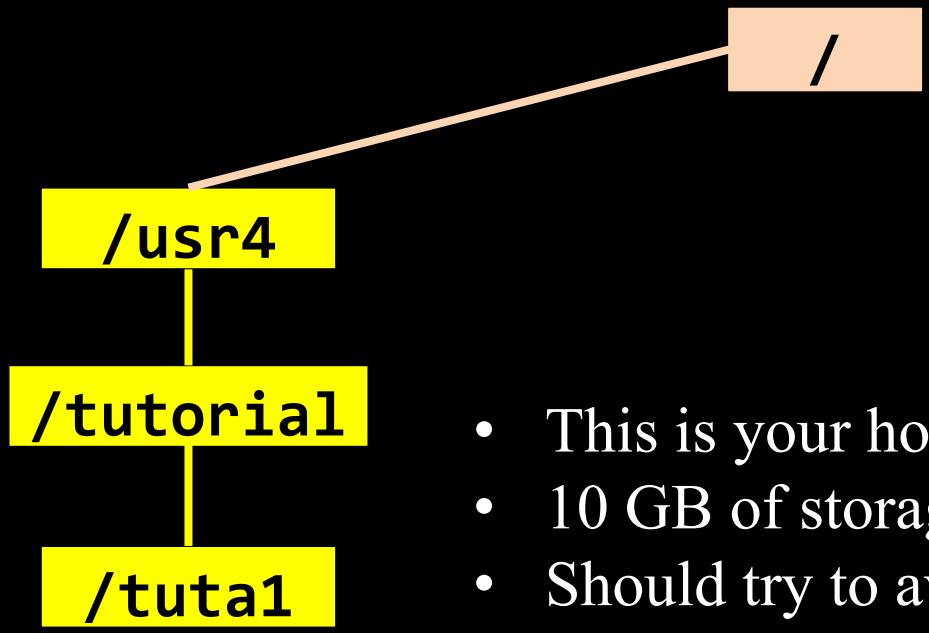
Unix

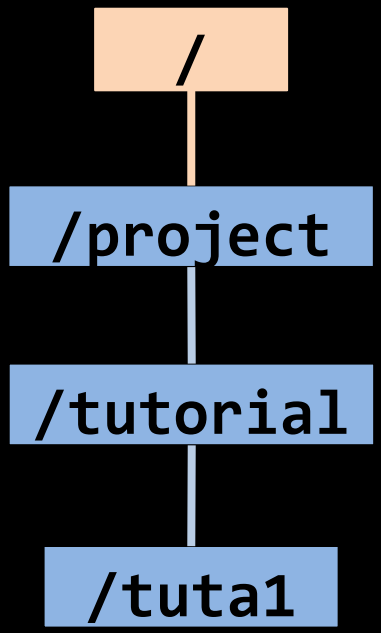

/
/usr4
/tutorial
/tuta1
/project
/tutorial
/tuta1
/projectnb
/tutorial
/tuta1

Unix



- This is your home directory
- 10 GB of storage
- Should try to avoid filling up this directory

Unix



- This is a backed-up project storage
- Backup in a separate location incase of physical damage
- Default 50GB of space, can increase to 200GB

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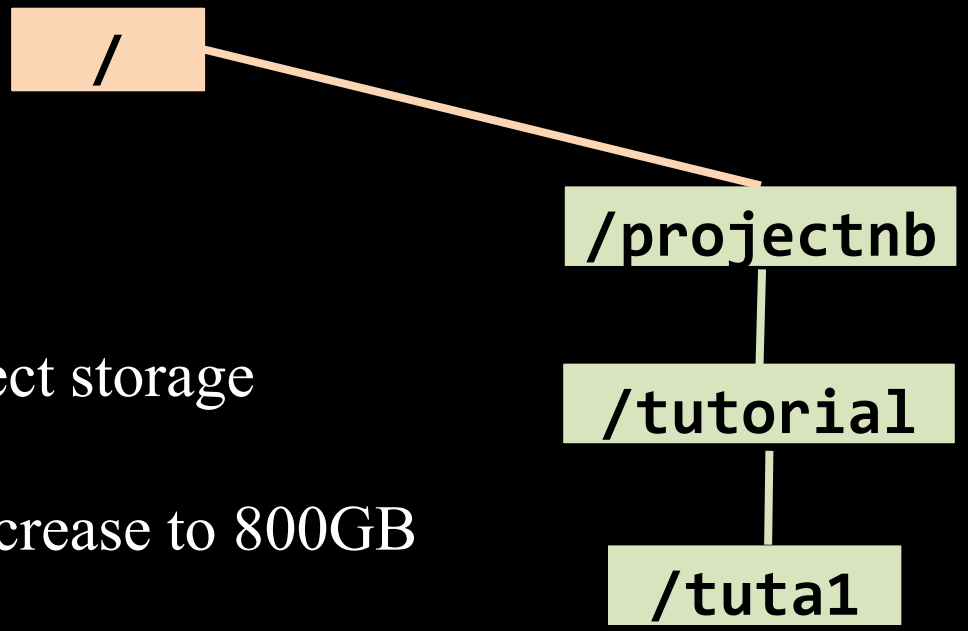
Unix



- This is a NOT backed-up project storage
- Local snapshots
- Default 50GB of space, can increase to 800GB

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Unix

```
[tuta1@scc-v01 ~]$ cd  /projectnb/tutorial
```

swap in your default group!

cd = change directory

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Unix

```
[tuta1@scc-v01 ~]$ mkdir  tuta1
```

swap in your username

mkdir = make a directory

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Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
 drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```

ls = list contents

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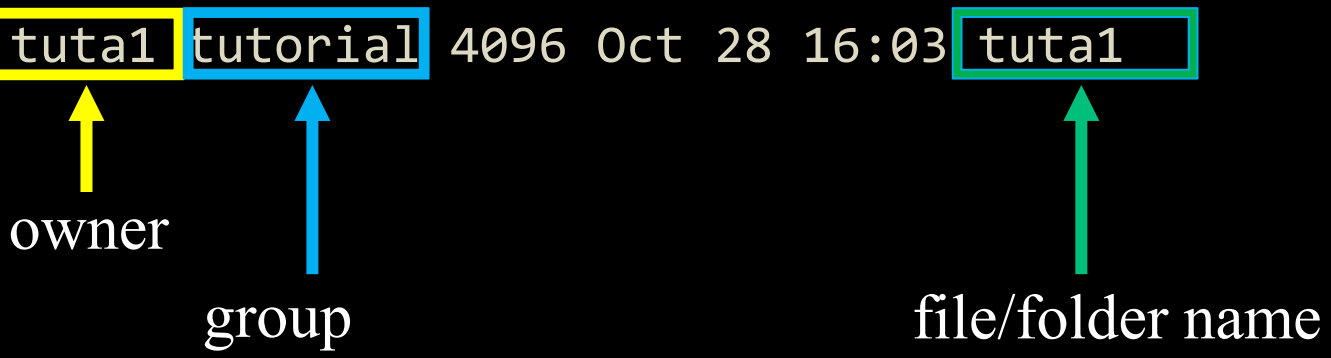
Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
 drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



ls = list contents

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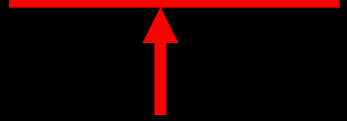
Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



ls = list contents

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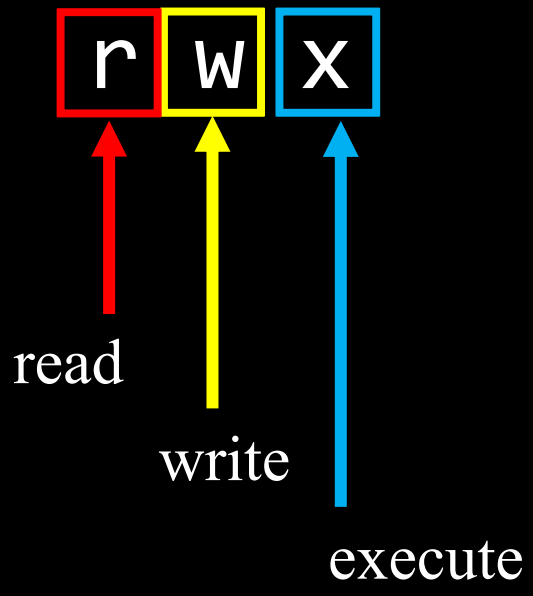
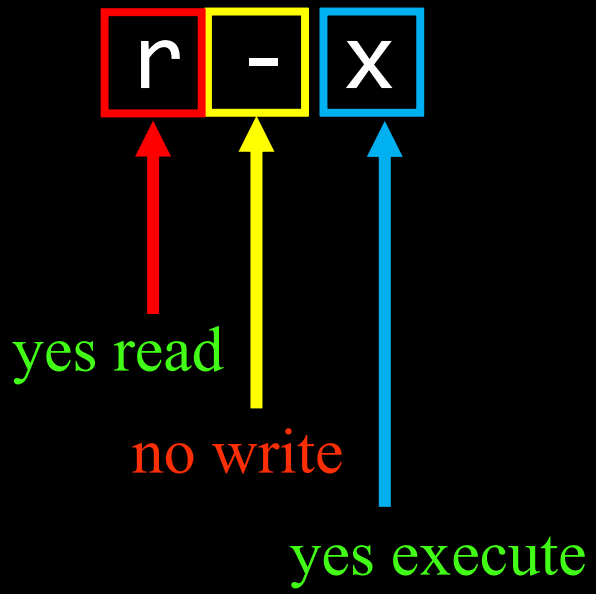
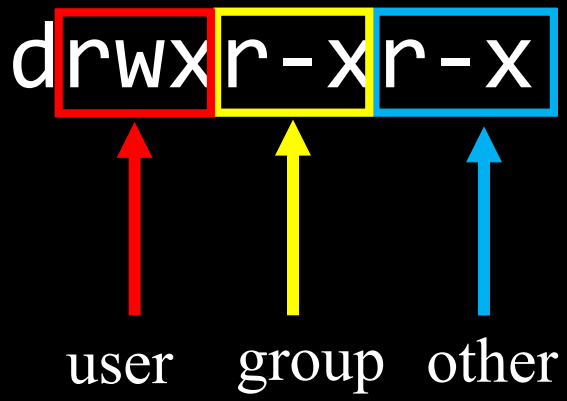
Unix



Unix

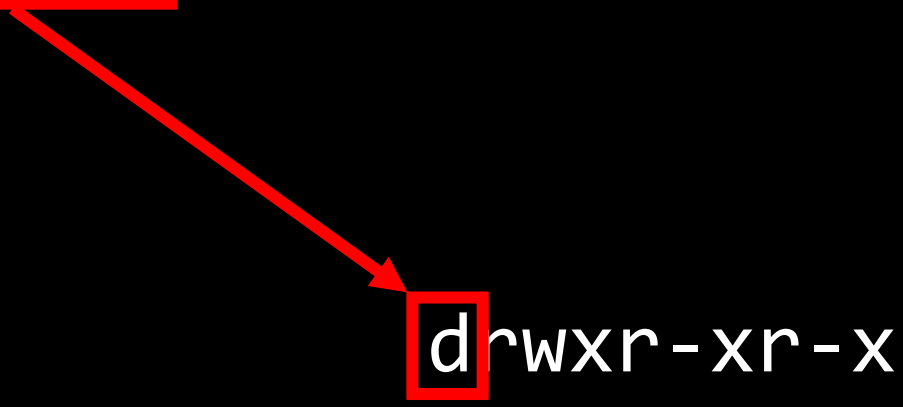


Unix



Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



Object Type

- d = directory
- - = file

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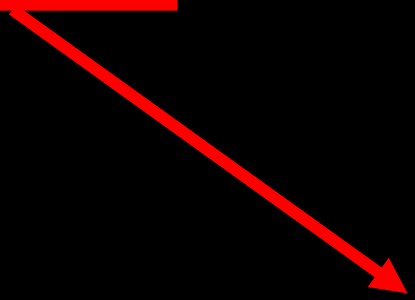
Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



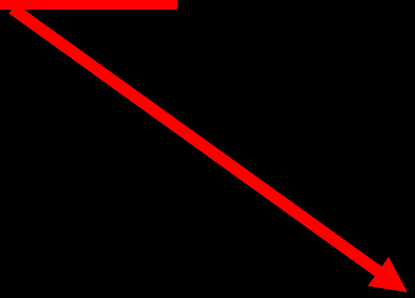
drwxr-xr-x

User/Owner Permissions:

- tuta1 is owner
- currently all enabled

Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



drwxr-xr-x

Group Permissions:

- tutorial is group
- read and execute are enabled
- write is not enabled

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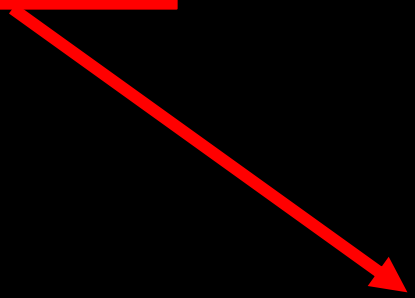
Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```



drwxr-xr-x

Other/World Permissions:

- read and execute are enabled
- write is not enabled

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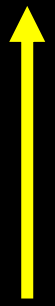
Unix

```
[tuta1@scc-v01 ~]$ ls  -l
total 1
 drwxr-xr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```

How can we change permissions?

Unix

```
[tuta1@scc-v01 ~]$ chmod  g+w  tuta1
```



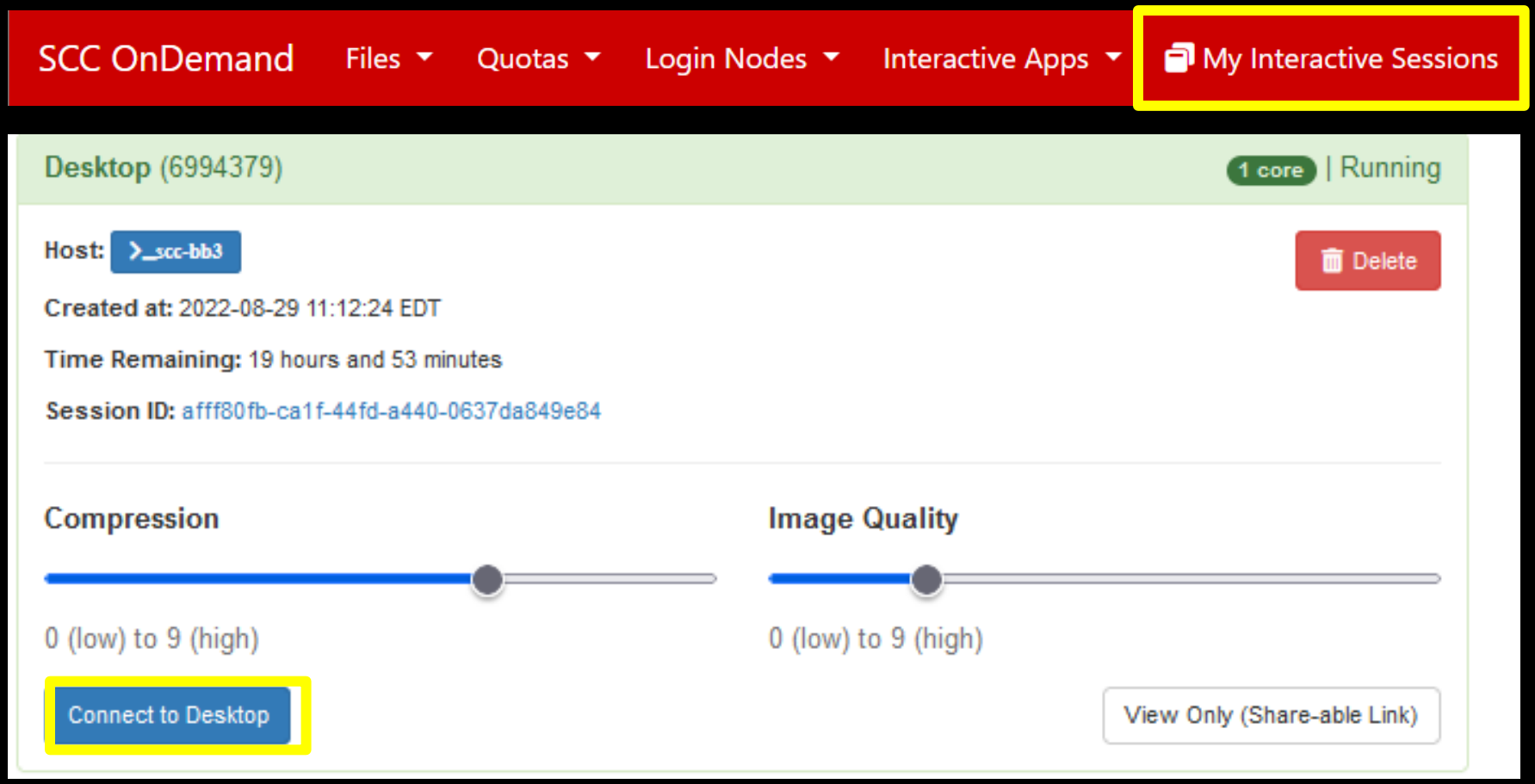
To group add write permissions

Unix

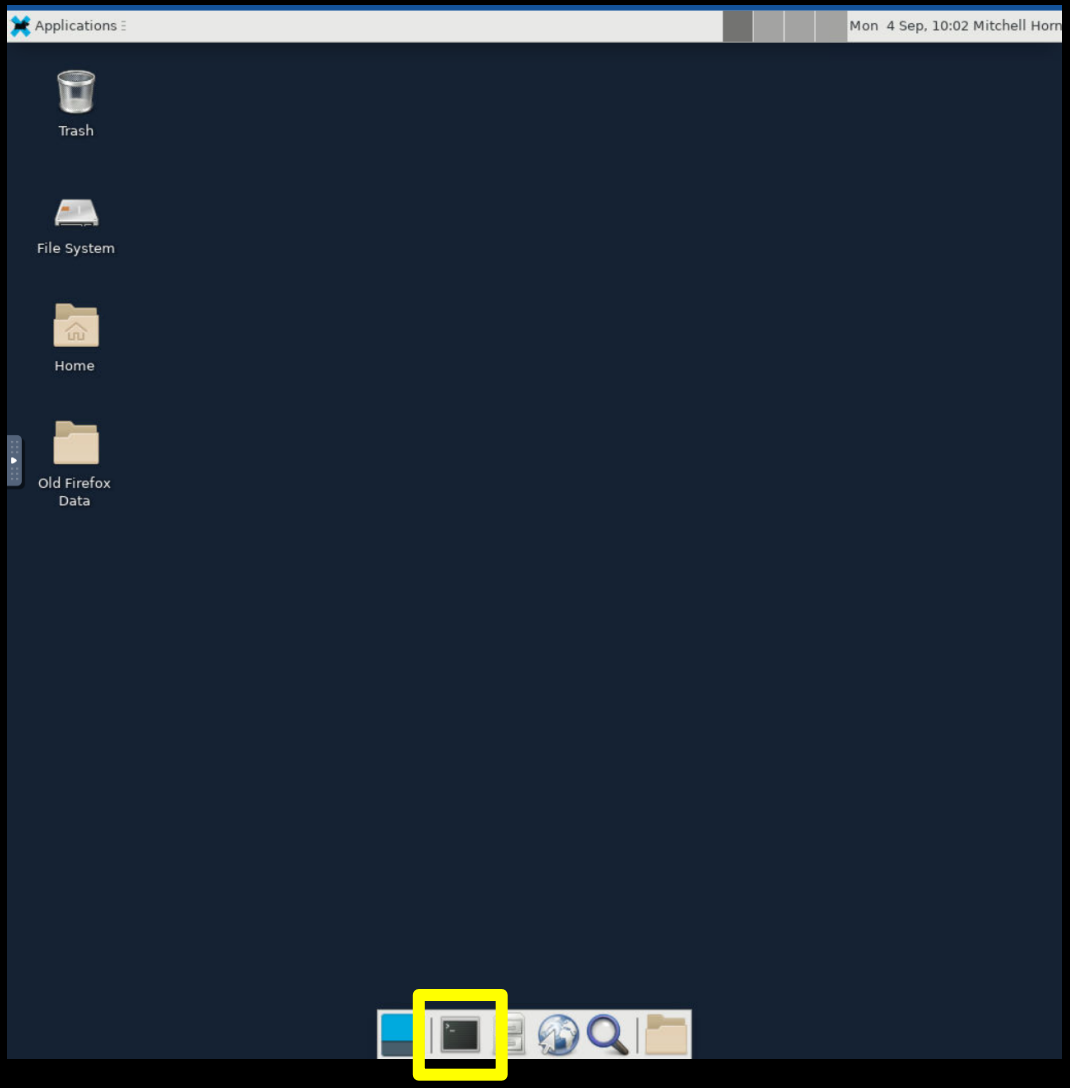
```
[tuta1@scc-v01 ~]$ ls  -l
total 1
 drwxrwxr-x 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1
```

yes write

OnDemand – Interactive Desktop



Connect to OnDemand



Unix

```
[]$ cd  /projectnb/tutorial/tuta1
```

swap in your username

cd = change directory

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Unix

```
[tuta1@scc-v01 tuta1]$ gedit  test.sh  &
```

gedit = graphical text editor

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Unix

```
1    echo “Welcome to the SCC!”
```

save; close (hit x in top-right)

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Unix

```
[tuta1@scc-v01 tuta1]$ chmod  u+x  test.sh
```

To user add execute permissions

Unix

```
[tuta0@scc-v01 tuta1]$ ./test.sh

  Welcome to the SCC!
```

Unix

```
[tuta1@scc-v01 tuta1]$ mv  test.sh  tuta1.sh
```

swap in your username

mv = move

- can also be used to rename files!

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Unix

```
[tuta1@scc-v01 tuta1]$ ls  -l
total 1
 -rwxr--r-- 3 tuta1 tutorial 4096 Oct 28 16:03 tuta1.sh
```

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Unix

```
[]$ cd  /projectnb/tutorial/tuta1
```

swap in your username

cd = change directory

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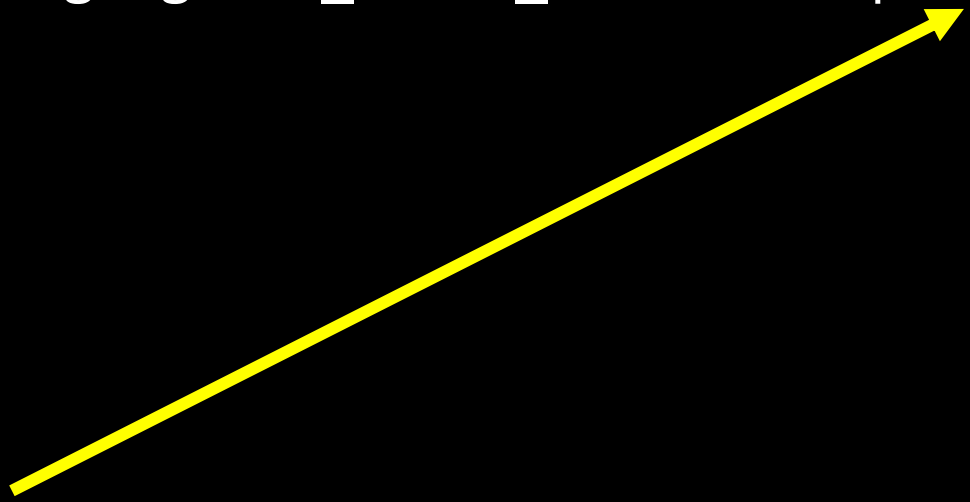
Wrangling Imaging Data

```
cp  /project/scv/examples/imaging/tut_neuro_scc/tut.zip  .
```



- `cp` = copy
- `.` = short-hand for current directory
- use [tab] key to autocomplete paths
  - `/project/scv/ex[tab]/im[tab]/tut_n[tab]/tut[tab]`

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Wrangling Imaging Data

```
[tuta1@scc-v01 tuta1]$ unzip  tut.zip
```

unzip the tutorial data

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Wrangling Imaging Data

```
[tuta1@scc-v01 tuta1]$ cd  tut
```

Wrangling Imaging Data

```
[tuta1@scc-v01 tuta1]$ ls  -l

-rwxrwsrwx  2 tuta1 tutorial     4096 Sep 11 12:54 bet.qsub
drwxrwsrwx  2 tuta1 tutorial     4096 Sep 11 12:54 dicom
```

list the contents of the tut directory

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Wrangling Imaging Data

```
[tuta1@scc-v01 tuta1]$ ls  -l  dicom

1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-97-10diwog.dcm
1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-98-2cfytv.dcm
1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-99-nkpf0x.dcm
…
```

list the contents of the dicom directory

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Wrangling Imaging Data

```
1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-97-10diwog.dcm
1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-98-2cfytv.dcm
1.3.12.2.1107.5.2.43.166024.30000022072919140806900000007-9-99-nkpf0x.dcm
…
```

- DICOM
  - Standard medical image format on most* imaging machines
  - Contains an image and metadata about the image (like most pictures)
  - The metadata contains information about the scan
  - Is not a conducive format for image processing

Wrangling Imaging Data

- NIfTI
  - Subject_001.nii, Subject_001.nii.gz
  - FreeSurfer, FSL, AFNI, SPM, CONN
- MGH/MGZ
  - Subject_001.mgh, Subject_001.mgh.gz, Subject_001.mgz
  - FreeSurfer
- BRIK & HEAD
  - Subject_001.BRIK & Subject_001.HEAD
  - AFNI
- IMG & HDR (Analyze Format)
  - Subject_001.img & Subject_001.hdr
  - SPM, FreeSurfer, FSL, AFNI

Wrangling Imaging Data

- Unpacking DICOMs
  - Reads through DICOM metadata to sort and stack slices/volumes into specified file format
- dcm2niix
  - MRICroGL
- ArcGet.py
- heudiconv
- dcmunpack / unpacksdcmdir
  - FreeSurfer
- spm_dicom_convert
  - SPM
- to3d
  - AFNI

Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  avail  |  less
```

ctrl+z to quit “less”

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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  avail  dcm2niix
```

ctrl+z to quit “less”

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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  load  dcm2niix
```

Module system to load software packages

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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  list

Currently Loaded Modules:
       1) dcm2niix/1.0.20220720
```

Module system to load software packages

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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ mkdir  nifti
```

Make a new folder called nifti

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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ dcm2niix  -o  nifti  dicom/*
```

* = short-hand for include everything

convert dicoms to nifti; and save them in the nifti directory

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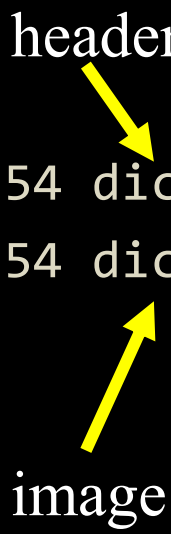
Software on the SCC

```
[tuta1@scc-v01 tuta1]$ ls  -l  nifti

-rw-r--r--  2 tuta1 tutorial    4096 Sep 11 12:54 dicom.json
-rw-r--r--  2 tuta1 tutorial    4096 Sep 11 12:54 dicom.nii
```



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Software on the SCC

Neuroimaging Suites

- FreeSurfer
- FSL
- AFNI
- SPM
- CONN
- ANTS

Neuroimaging Tools

- MRIcroGL
- MRIcron
- Osirix
- Nipype
- MRIQC

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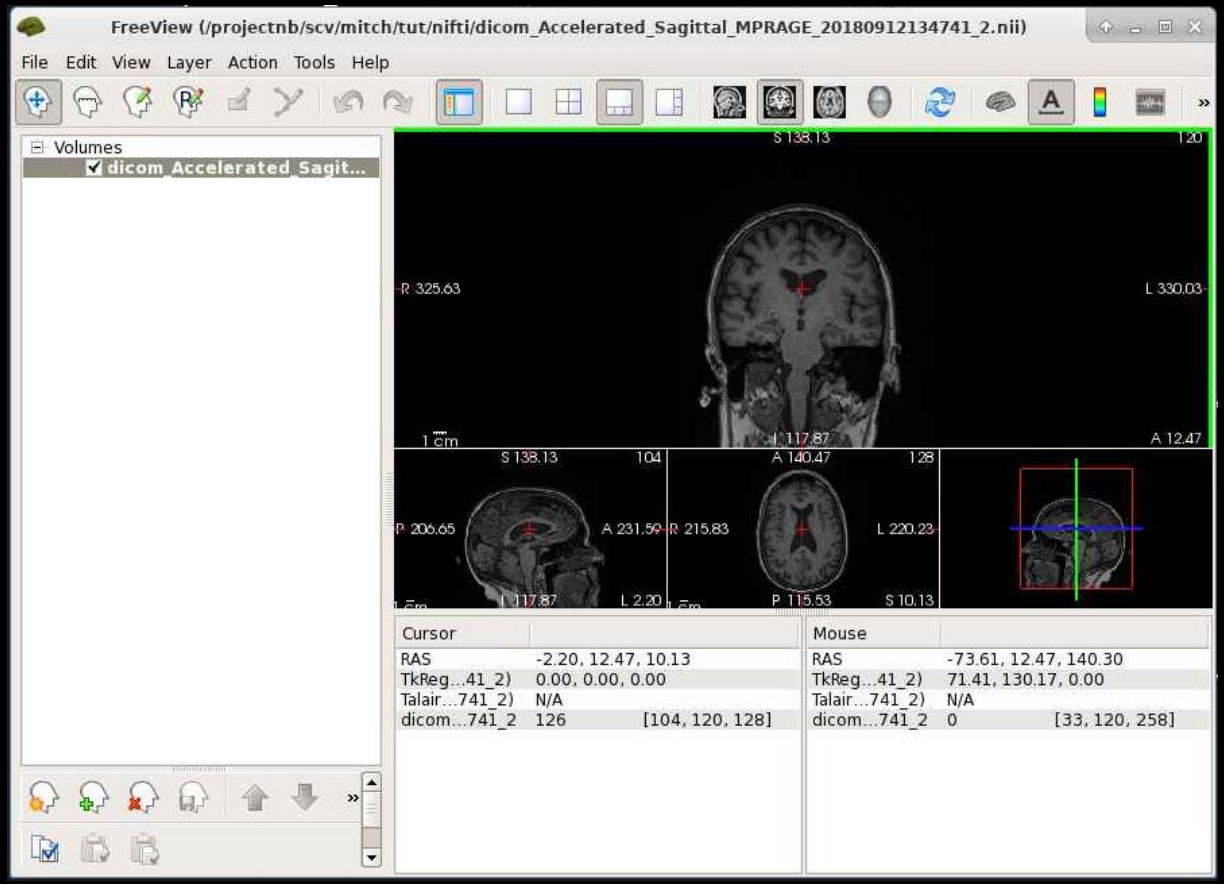
Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  load  freesurfer
```

Software on the SCC

```
[tuta1@scc-v01 tuta1]$ freeview  nifti/*.nii
```



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Software on the SCC

```
[tuta1@scc-v01 tuta1]$ module  purge
```

```
[tuta1@scc-v01 tuta1]$ module  list
```

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Topics

- Get On the SCC
- What/Where/How the SCC?
- OnDemand
- Unix
- Wrangling Imaging Data
- XNAT
- Using the Batch System
- Useful Tools

Using the Interactive Node

- 1 Computer - Non-Parallelized (~80 Hours for 8 Subjects):

- SCC - Parallelized (~5 Hours for 8 Subjects):

https://rcs.bu.edu/examples/imaging/freesurfer/

Using the Interactive Node

```
[tuta1@scc-v01 tuta1]$ pwd
/projectnb/tutorial/tuta1/tut
```

Check to make sure we are in the “tut” directory!

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Using the Interactive Node

```
[tuta1@scc-v01 tuta1]$ module load fsl/6.0.4
```

```
[tuta1@scc-v01 tuta1]$ module list
Currently Loaded Modules:
  1) fsl/6.0.4
```

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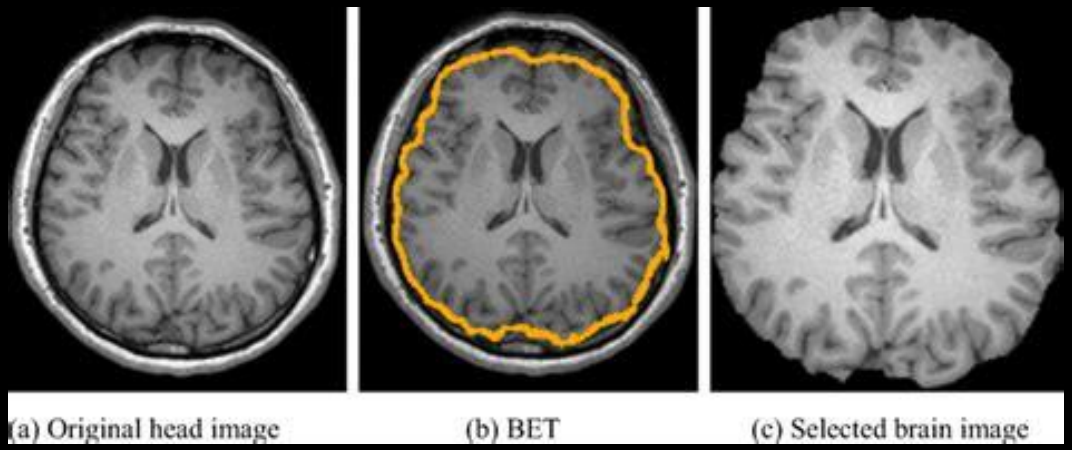
Using the Interactive Node

bet = Brain Extraction Tool

```
[~]$ bet input output
```



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Using the Interactive Node

```
[tuta1@scc-v01 tuta1]$ bet nifti/dicom[tab].nii  nifti/ss.nii
```

`[tab]` = use [tab] button to autocomplete filenames!

Using the Interactive Node

```
[tuta1@scc-v01 tuta1]$ ls  -l  nifti

-rw-r--r--  2 tuta1 tutorial    4096 Sep 11 12:54 dicom.json
-rw-r--r--  2 tuta1 tutorial    4096 Sep 11 12:54 dicom.nii
-rw-r--r--  2 tuta1 tutorial    4096 Sep 11 12:54 ss.nii.gz
```

Using the Interactive Node

```
[tuta1@scc-v01 tuta1]$ module  load  freesurfer
```

```
[tuta1@scc-v01 tuta1]$ freeview  nifti/*.nii  nifti/*.nii.gz
```

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Using the Batch System

```
[tuta1@scc-v01 tuta1]$ gedit  bet.qsub  &
```

Open the bet.qsub file in gedit

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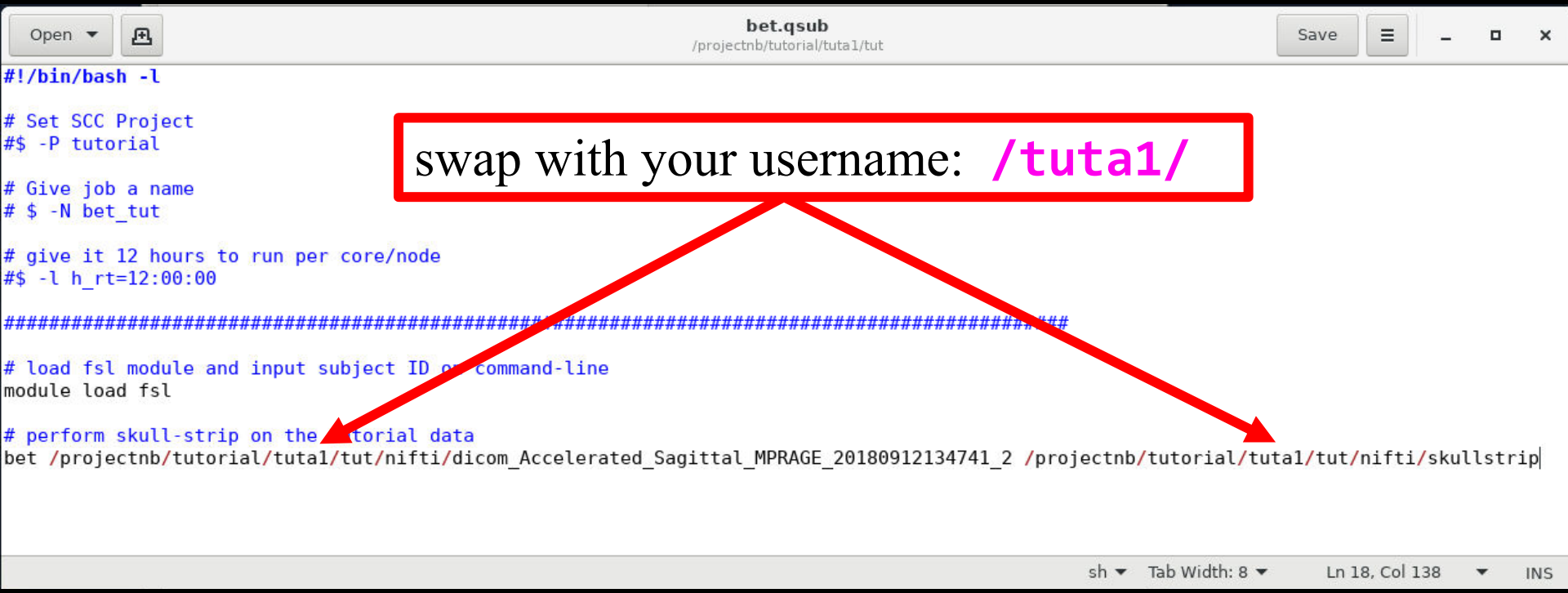
Using the Batch System



Submitting a Job to the SCC

```
[tuta1@scc-v01 tuta1]$ qsub  bet.qsub
Your job 1041461 (“bet.qsub") has been submitted
```

Submit job with qsub

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qsub Details

- Submit non-interactive batch jobs using **qsub**

  qsub *[options]* ***command*** *[arguments]*

- Setting default **qsub** options using a .sge_request file:

  http://www.bu.edu/tech/support/research/system-usage/running-jobs/advanced-batch/#sge_request

- **http://www.bu.edu/tech/support/research/system-usage/running-jobs/submitting-jobs/**

qsub options

General Directives	
Directive	**Description**
-l h_rt=*hh:mm:ss*	Hard run time limit in *hh:mm:ss* format. The default is 12 hours.
-P *project_name*	Project to which this jobs is to be assigned. This directive is **mandatory** for all users associated with any Med.Campus project.
-N *job_name*	Specifies the job name. The default is the script or command name.
-o *outputfile*	File name for the stdout output of the job.
-e *errfile*	File name for the stderr output of the job.
-j y	Merge the error and output stream files into a single file.
-m *b|e|a|s|n*	Controls when the batch system sends email to you. The possible values are – when the job begins (b), ends (e), is aborted (a), is suspended (s), or never (n) – default.
-M *user_email*	Overwrites the default email address used to send the job report.
-V	All current environment variables should be exported to the batch job.
-v *env=value*	Set the runtime environment variable *env* to *value*.
-hold_jid *job_list*	Setup job dependency list. *job_list* is a comma separated list of job ids and/or job names which must complete before this job can run. See Advanced Batch System Usage for more information.

qsub options cont.

Directives to request SCC resources	
Directive	**Description**
-l h_rt=*hh:mm:ss*	Hard run time limit in *hh:mm:ss* format. The default is 12 hours.
-l mem_total =*#G*	Request a node that has at least this amount of memory. Current possible choices include 94G, 125G, 252G, 504G, and 1000G
-l mem_per_core =*#G*	Request a node that has at least this amount of memory per core. Current possible choices include 3G, 4G, 8G, 12G, 16G, 18G and 28G
-pe omp *N*	Request multiple slots for Shared Memory applications (OpenMP, pthread). This option can also be used to reserve a larger amount of memory for the application. *N* can vary 1-28, 36.
-pe mpi_#_tasks_per_node *N*	Select multiple nodes for an MPI job. Number of tasks can be 4, 8, 12, 16, or 28 and *N* must be a multiple of this value. See Running Parallel Batch Jobs for more information.
-t *N*	Submit an Array Job with *N* tasks. N can be up to 75,000. For more information see Array Jobs
-l cpu_arch=*ARCH*	Select a processor architecture (broadwell, haswell, ivybridge, ...). See Technical Summary for all available choices.
-l cpu_type=*TYPE*	Select a processor type (X5650, X5670, X5675, etc.) See Technical Summary for all available choices.
-l gpus=*G/C*	Requests a node with GPUs. *G/C* specifies the number of GPUs per CPU requested and should be expressed as a decimal number. See GPU Computing for more information.
-l gpu_type=*GPUMODEL*	Current choices for *GPUMODEL* are M2070, K40m, and P100.
-l gpu_c=*CAPABILITY*	Specify minimum GPU capability. Current choices for *CAPABILITY* are 2.0, 3.5, and 6.0

Checking Job Status

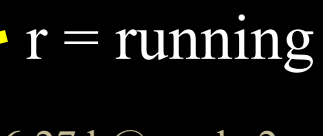
```
[tuta1@scc-v01 tuta1]$ qstat  -u  tuta1
```

swap in your username

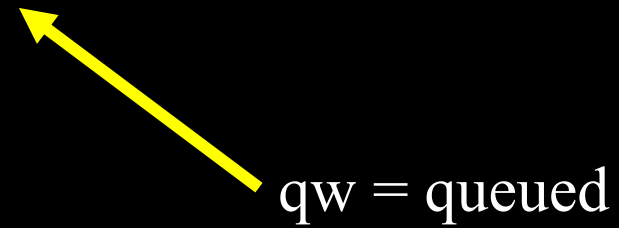
Check status of job

Checking Job Status

```
[tuta1@scc-v01 tuta1]$ qstat  -u  tuta1
```




```
7238828 0.14071 ood-deskto   tuta1      r     09/12/2022 09:46:27 b@scc-bc2.scc.bu.edu   1
7243957 0.00000 bet.qsub     tuta1      qw    09/12/2022 14:47:20                        1
```



Check status of job

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qsub output

- The job should run soon and produce an output file:

```
[tuta1@scc1 tut]$ cat bet.qsub.o1041461
```

- There will also be an error file which should be empty:

```
[tuta1@scc1 tut]$ cat bet.qsub.e1041461
```

Topics

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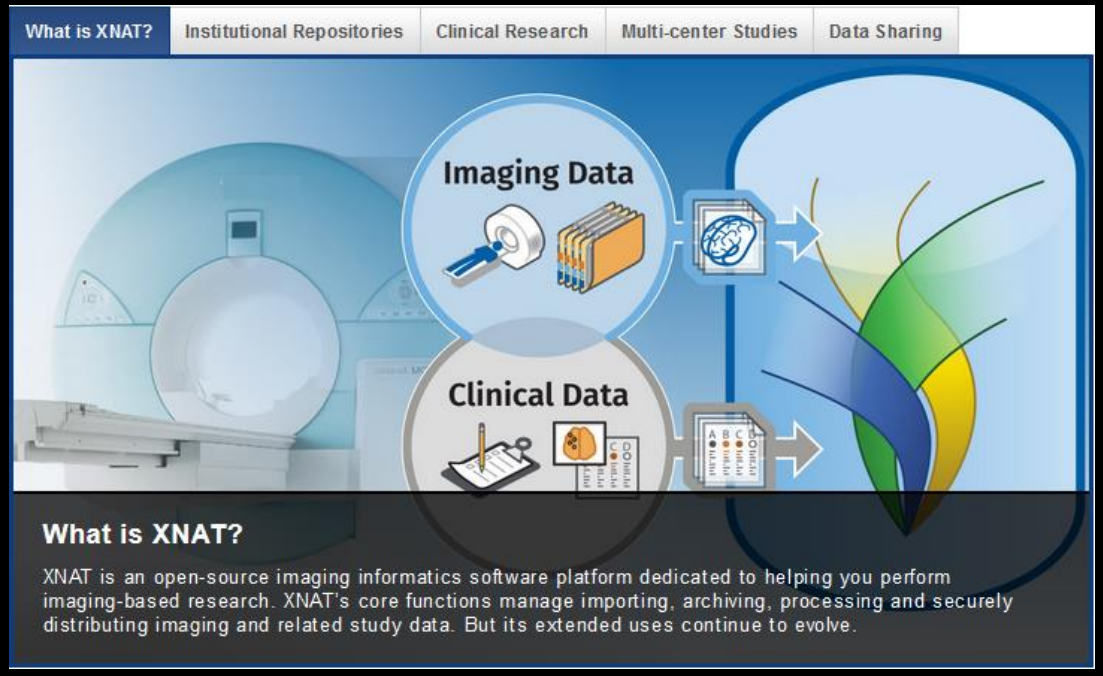
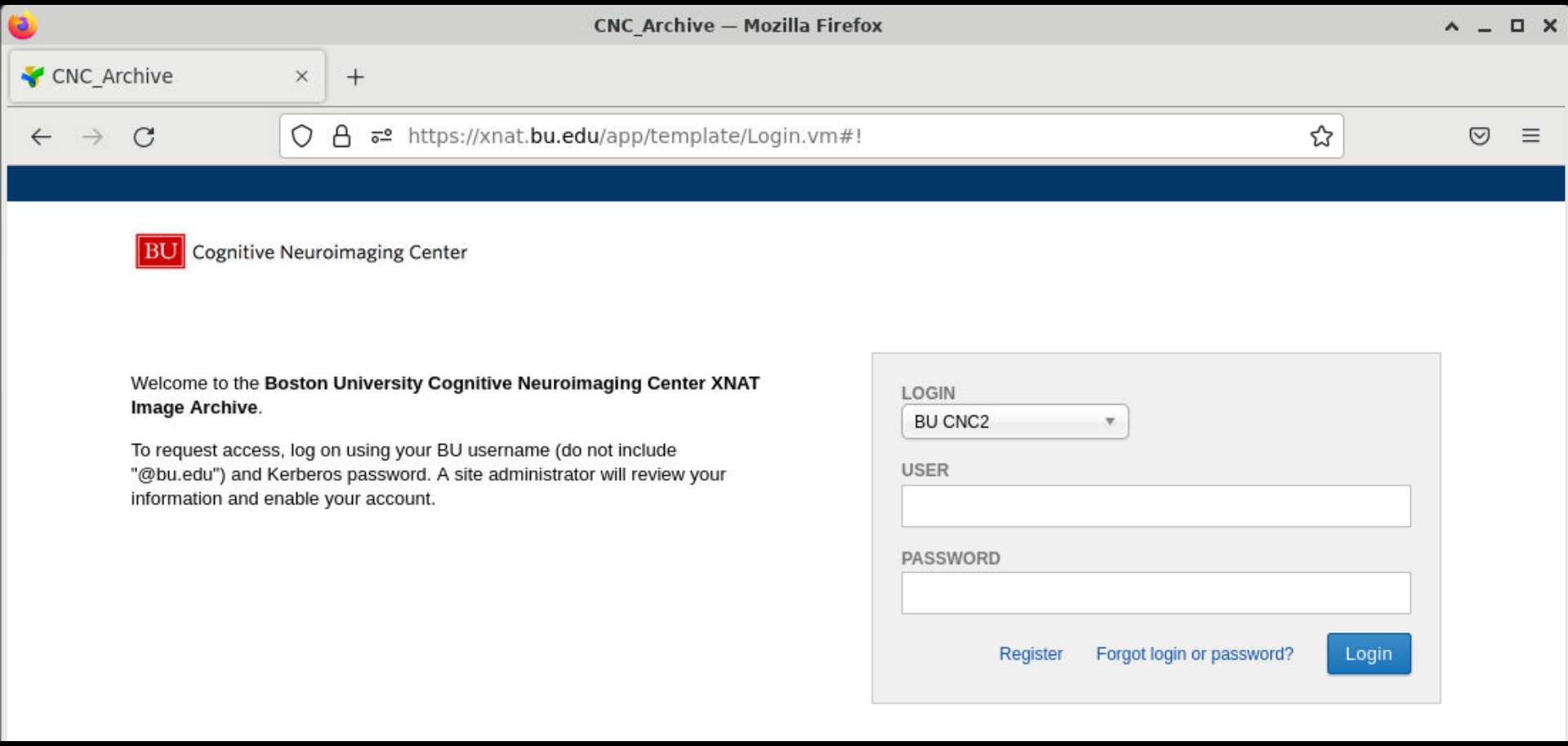
XNAT

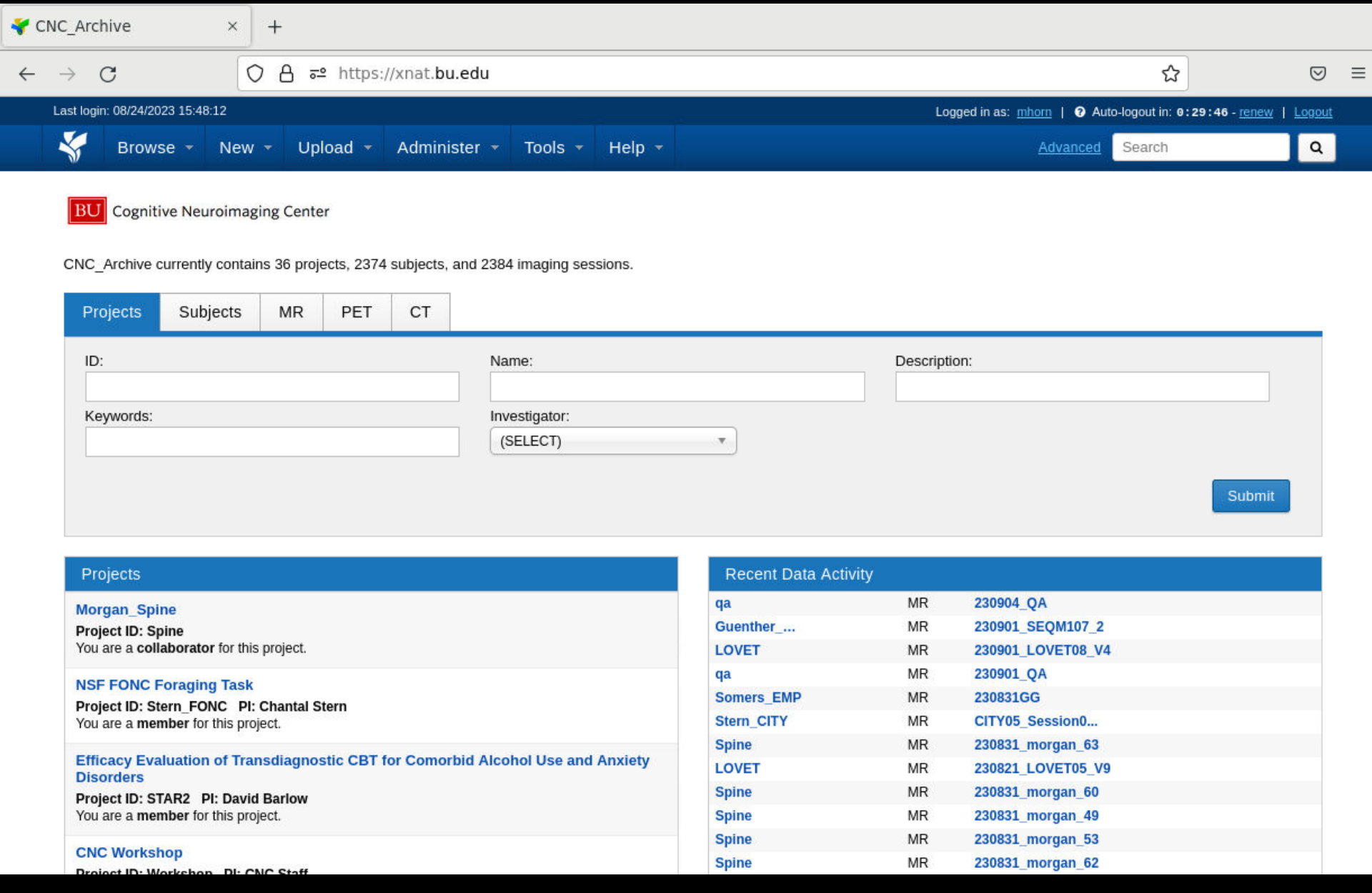
- Software platform that will store CNC neuroimaging data
- Live Upload from MRI Scanner to XNAT
- Inspect/Download raw data for artifacts before processing in Web API (Demo)



XNAT


CNC_Archive — Mozilla Firefox
CNC_Archive
https://xnat.bu.edu/app/template/Login.vm#!
BU Cognitive Neuroimaging Center
Welcome to the Boston University Cognitive Neuroimaging Center XNAT Image Archive.
To request access, log on using your BU username (do not include "@bu.edu") and Kerberos password. A site administrator will review your information and enable your account.
LOGIN
BU CNC2
USER
PASSWORD
Register
Forgot login or password?
Login

XNAT


CNC_Archive
https://xnat.bu.edu
Last login: 08/24/2023 15:48:12
Logged in as: mhorn | Auto-logout in: 0:29:46 - renew | Logout
Browse
New
Upload
Administer
Tools
Help
Advanced
Search
BU Cognitive Neuroimaging Center
CNC_Archive currently contains 36 projects, 2374 subjects, and 2384 imaging sessions.
Projects
Subjects
MR
PET
CT
ID:
Name:
Description:
Keywords:
Investigator:
(SELECT)
Submit
Projects
Morgan_Spine
Project ID: Spine
You are a collaborator for this project.
NSF FONC Foraging Task
Project ID: Stern_FONC PI: Chantal Stern
You are a member for this project.
Efficacy Evaluation of Transdiagnostic CBT for Comorbid Alcohol Use and Anxiety Disorders
Project ID: STAR2 PI: David Barlow
You are a member for this project.
CNC Workshop
Recent Data Activity
qa MR 230904_QA
Guenther_... MR 230901_SEQM107_2
LOVET MR 230901_LOVET08_V4
qa MR 230901_QA
Somers_EMP MR 230831GG
Stern_CITY MR CITY05_Session0...
Spine MR 230831_morgan_63
LOVET MR 230821_LOVET05_V9
Spine MR 230831_morgan_60
Spine MR 230831_morgan_49
Spine MR 230831_morgan_53
Spine MR 230831_morgan_62

Downloading from XNAT

```
[~]$ module  load  python3/3.8.10
[~]$ module  load  yaxil/0.9.0
```

Downloading from XNAT

```
[~]$ ArcGet.py  –a  xnat  –l  220801_Rise_demo_01  –p  Workshop  -o .

Enter XNAT passphrase:
INFO:/share/pkg.7/yaxil/0.6.5_dwi_beta/install/bin/ArcGet.py:downloading scans
1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22
reading response data: done.
```

Topics

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Additional Web Resources

- Research Computing Support Pages

https://www.bu.edu/tech/support/research/

- Running Jobs on the SCC

https://www.bu.edu/tech/support/research/system-usage/running-jobs/

- Software Packages on the SCC

https://www.bu.edu/tech/support/research/software-and-programming/software-and-applications/

1. Please open a web browser and:
2. Google “rcs tutorial evaluation”
3. Click 1st link
   http://scv.bu.edu/survey/tutorial_evaluation.html
4. Fill out the survey!