ilifu

IDIA

ilifu Online Training

Jeremy Smith
User Training Workshop – Introduction to ilifu
4 April 2023

Topics

- Introduction to the ilifu research facility services
- Directory structure
- Software environment
    - Singularity containers
    - Modules
- Using JupyterHub
- Introduction to Slurm

Getting help

- Support contact

  support@ilifu.ac.za

- User documentation

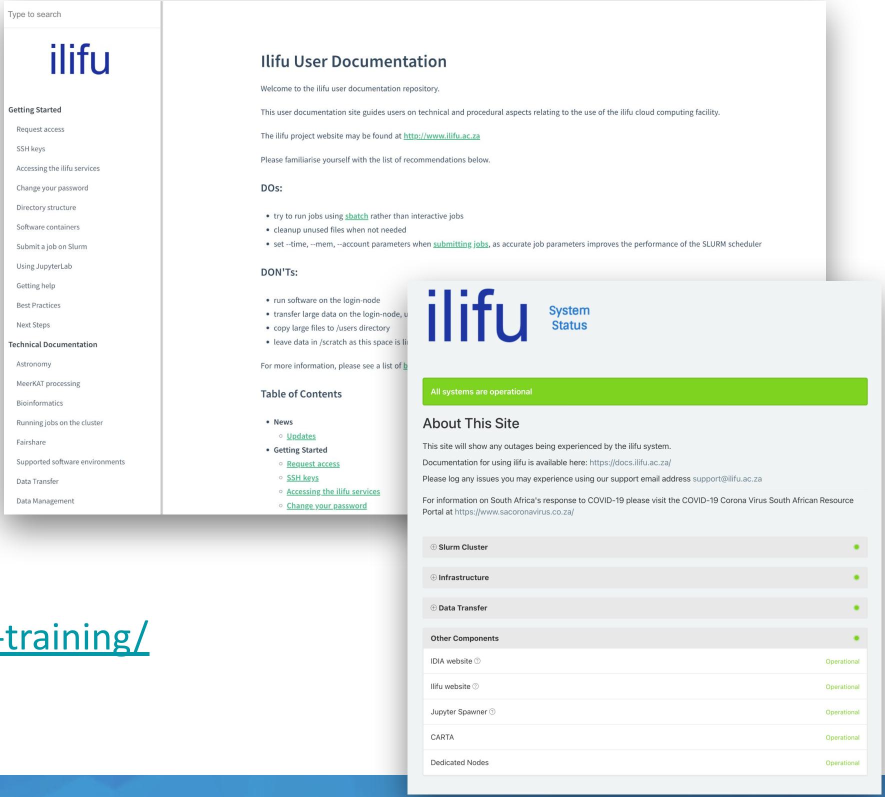
  http://docs.ilifu.ac.za/#/

- Ilifu System Status

  https://status.ilifu.ac.za/

- Training videos

  https://www.ilifu.ac.za/latest-training/



Type to search

ilifu

Getting Started

- Request access
- SSH keys
- Accessing the ilifu services
- Change your password
- Directory structure
- Software containers
- Submit a job on Slurm
- Using JupyterLab
- Getting help
- Best Practices
- Next Steps

Technical Documentation

- Astronomy
- MeerKAT processing
- Bioinformatics
- Running jobs on the cluster
- Fairshare
- Supported software environments
- Data Transfer
- Data Management

Ilifu User Documentation

Welcome to the ilifu user documentation repository.

This user documentation site guides users on technical and procedural aspects relating to the use of the ilifu cloud computing facility.

The ilifu project website may be found at http://www.ilifu.ac.za

Please familiarise yourself with the list of recommendations below.

DOs:

- try to run jobs using sbatch rather than interactive jobs
- cleanup unused files when not needed
- set --time, --mem, --account parameters when submitting jobs, as accurate job parameters improves the performance of the SLURM scheduler

DON'Ts:

- run software on the login-node
- transfer large data on the login-node, u
- copy large files to /users directory
- leave data in /scratch as this space is li

For more information, please see a list of b

Table of Contents

- **News**
  - Updates
- **Getting Started**
  - Request access
  - SSH keys
  - Accessing the ilifu services
  - Change your password

ilifu System Status

All systems are operational

About This Site

This site will show any outages being experienced by the ilifu system.

Documentation for using ilifu is available here: https://docs.ilifu.ac.za/

Please log any issues you may experience using our support email address support@ilifu.ac.za

For information on South Africa's response to COVID-19 please visit the COVID-19 Corona Virus South African Resource Portal at https://www.sacoronavirus.co.za/

⊕ **Slurm Cluster**	●
⊕ **Infrastructure**	●
⊕ **Data Transfer**	●
Other Components	●
IDIA website ⓘ	Operational
Ilifu website ⓘ	Operational
Jupyter Spawner ⓘ	Operational
CARTA	Operational
Dedicated Nodes	Operational

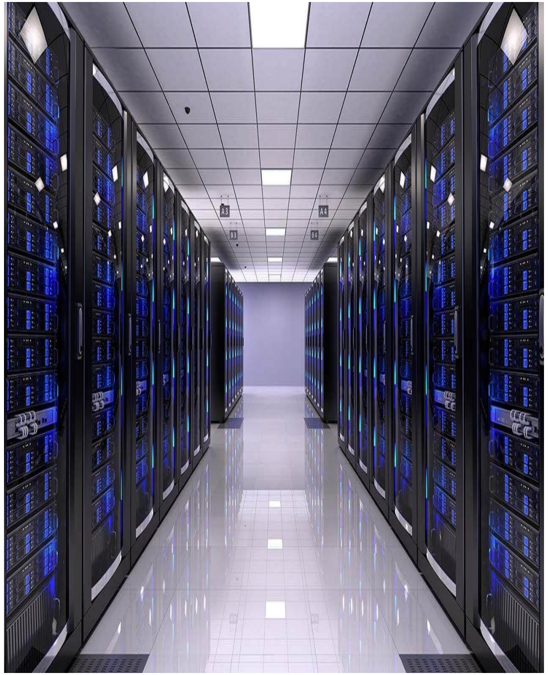
High Performance Computing

Combining power of distributed computers

- Collection of servers (computers)
- Connected by fast local network

Some terminology

- Servers also referred to as nodes
- Group of nodes is a cluster



ilifu

ilifu Research Facility

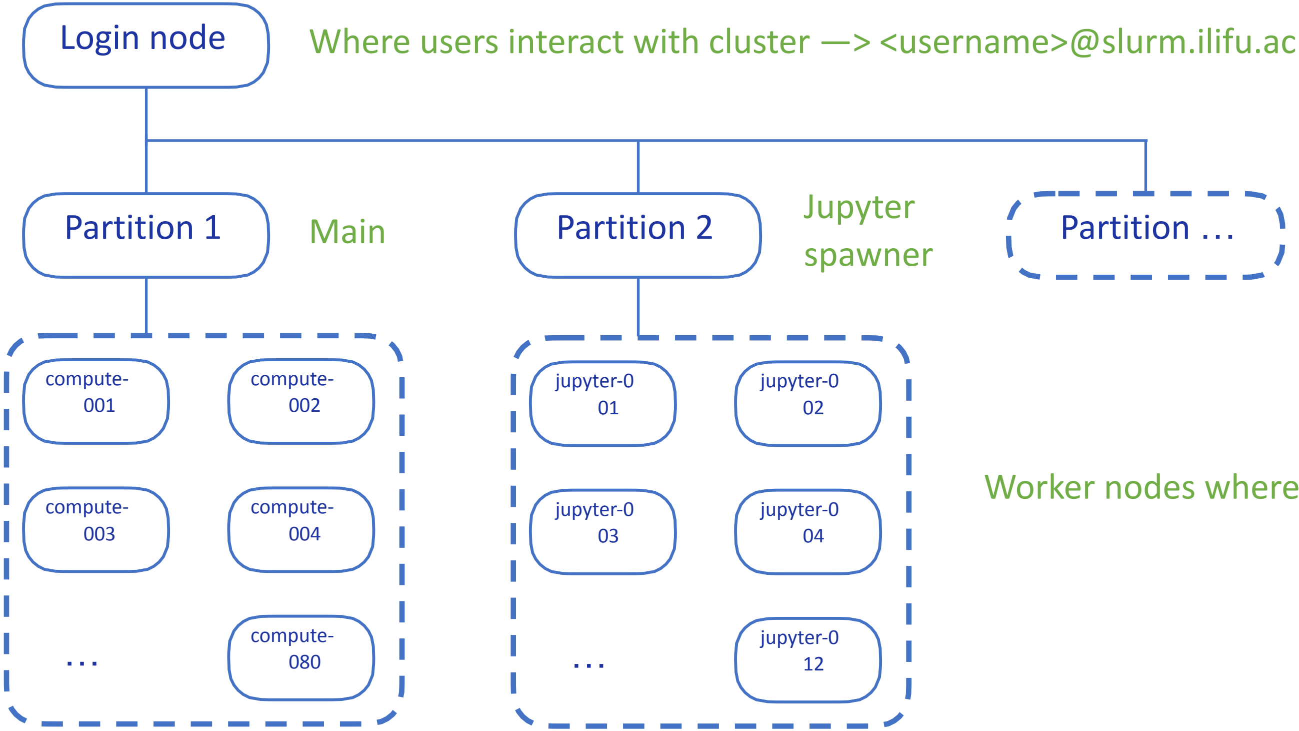
IDIA

Cloud-based infrastructure for data-intensive research

Remote access to compute and storage resources:

- Support variety of different scientific projects and requirements
- Flexible compute environment
- Data management: storage, transfer

ilifu Research Facility



Where users interact with cluster —> <username>@slurm.ilifu.ac.za

Main

Jupyter spawner

Other partitions

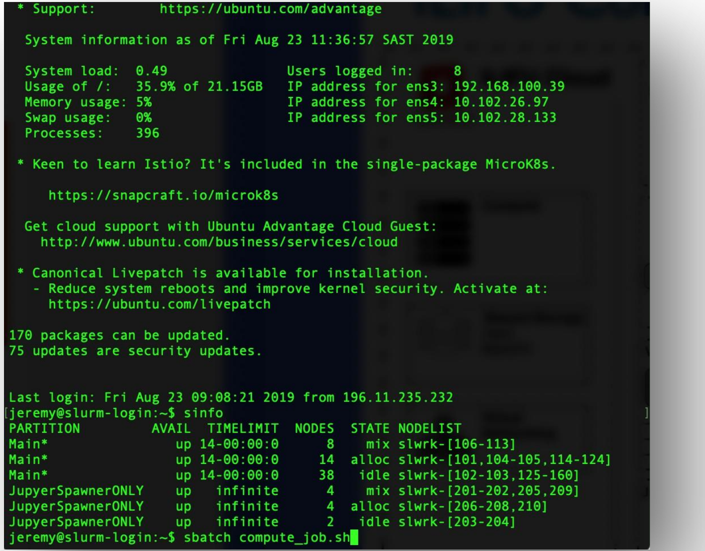
Worker nodes where our jobs run

Software we use

- Job Scheduler to manage resources - Slurm
- JupyterHub service - development environment
- Containerised software environment - Singularity
- Other services: data transfer, CARTA

Computing environment - interface

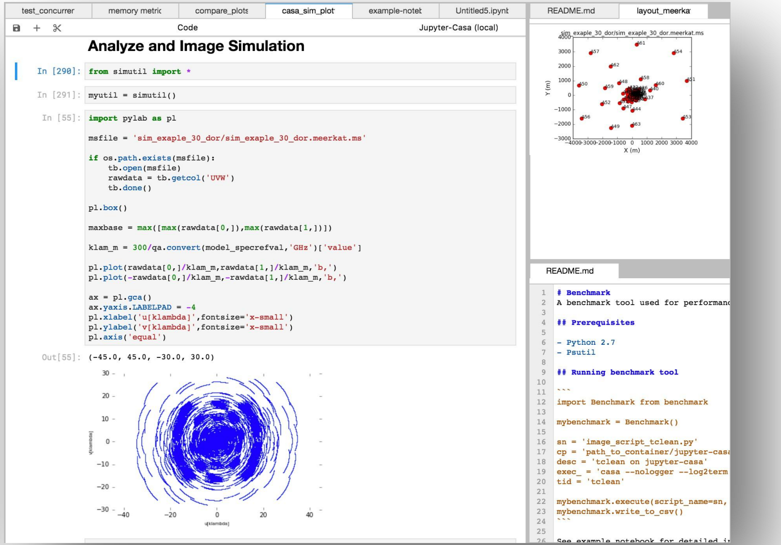
ssh - shell terminal



```
 * Support:        https://ubuntu.com/advantage

  System information as of Fri Aug 23 11:36:57 SAST 2019

  System load:  0.49              Users logged in:     8
  Usage of /:   35.9% of 21.15GB  IP address for ens3: 192.168.100.39
  Memory usage: 5%                IP address for ens4: 10.102.26.97
  Swap usage:   0%                IP address for ens5: 10.102.28.133
  Processes:    396

 * Keen to learn Istio? It's included in the single-package MicroK8s.

     https://snapcraft.io/microk8s

  Get cloud support with Ubuntu Advantage Cloud Guest:
    http://www.ubuntu.com/business/services/cloud

 * Canonical Livepatch is available for installation.
   - Reduce system reboots and improve kernel security. Activate at:
     https://ubuntu.com/livepatch

170 packages can be updated.
75 updates are security updates.


Last login: Fri Aug 23 09:08:21 2019 from 196.11.235.232
jeremy@slurm-login:~$ sinfo
PARTITION         AVAIL  TIMELIMIT  NODES  STATE NODELIST
Main*                up 14-00:00:0      8    mix slwrk-[106-113]
Main*                up 14-00:00:0     14  alloc slwrk-[101,104-105,114-124]
Main*                up 14-00:00:0     38   idle slwrk-[102-103,125-160]
JupyerSpawnerONLY    up   infinite      4    mix slwrk-[201-202,205,209]
JupyerSpawnerONLY    up   infinite      4  alloc slwrk-[206-208,210]
JupyerSpawnerONLY    up   infinite      2   idle slwrk-[203-204]
jeremy@slurm-login:~$ sbatch compute_job.sh
```

ssh <username>@slurm.ilifu.ac.za

JupyterHub



Analyze and Image Simulation

```
In [290]: from simutil import *

In [291]: myutil = simutil()

In [55]:  import pylab as pl

          msfile = 'sim_exaple_30_dor/sim_exaple_30_dor.meerkat.ms'

          if os.path.exists(msfile):
              tb.open(msfile)
              rawdata = tb.getcol('UVW')
              tb.done()

          pl.box()

          maxbase = max([max(rawdata[0,]),max(rawdata[1,])])

          klam_m = 300/qa.convert(model_specrefval,'GHz')['value']

          pl.plot(rawdata[0,]/klam_m,rawdata[1,]/klam_m,'b,')
          pl.plot(-rawdata[0,]/klam_m,-rawdata[1,]/klam_m,'b,')

          ax = pl.gca()
          ax.yaxis.LABELPAD = -4
          pl.xlabel('u[klambda]',fontsize='x-small')
          pl.ylabel('v[klambda]',fontsize='x-small')
          pl.axis('equal')

Out[55]:  (-45.0, 45.0, -30.0, 30.0)
```

```
# Benchmark
A benchmark tool used for performanc

## Prerequisites

- Python 2.7
- Psutil

## Running benchmark tool

```
import Benchmark from benchmark

mybenchmark = Benchmark()

sn = 'image_script_tclean.py'
cp = 'path_to_container/jupyter-casa
desc = 'tclean on jupyter-casa'
exec_ = 'casa --nologger --log2term
tid = 'tclean'

mybenchmark.execute(script_name=sn,
mybenchmark.write_to_csv()
```

See example notebook for detailed i
```

https://jupyter.ilifu.ac.za

ilifu

Computing environment - ssh

Your SSH key

- Used in the SSH (Secure Shell) protocol
- Authentication method for gaining access to encrypted connecting between systems
- Use connection to manage system remotely
- We need your SSH public key so our system knows to let you in

Compute environment - ssh

Generating SSH key

- If you don’t already have one
- New compute/formatted existing computer

GitHub docs on key generation:

https://docs.github.com/en/github/authenticating-to-github/connecting-to-github-with-ssh/generating-a-new-ssh-key-and-adding-it-to-the-ssh-agent

Directory Structure

Common areas:

- /users
  - limited storage shared among all users, for scripts and small files – don’t place data here, capping /users storage capacity can prevent access to the cluster for all users.
- /scratch3/users
  - directory space for processing data, temporary storage only, i.e. use this space during processing, and then clear all files immediately after processing. Remove unnecessary data and move data that you want to keep to project folder.

Remaining storage separated by group: IDIA, CBio, ilifu

Directory Structure

IDIA structure:

- /idia/users
  - user's private work directory, may store data products that are not ready to move to shared project space
- /idia/projects
  - project specific directories. These directories are for sharing data and resources within project groups. Raw data associated with a project will also be available from the project folder. Raw data should always be read-only.
- /idia/software
  - software containers and the IDIA Pipelines software is stored here

Directory Structure

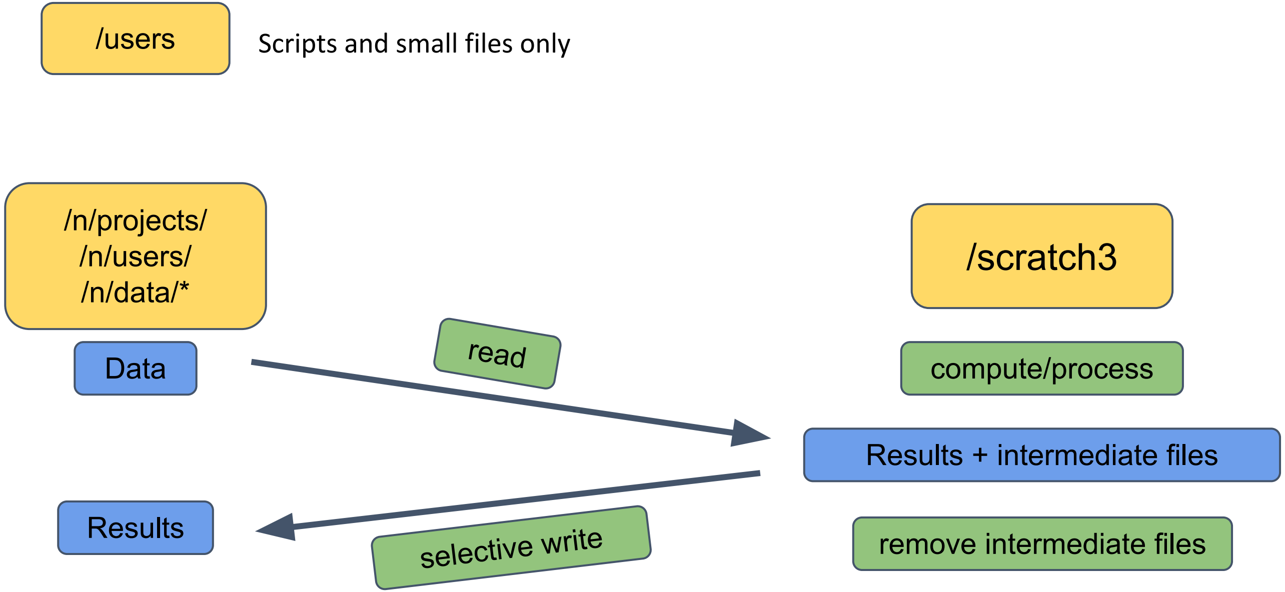
Similar structure for /cbio and /ilifu groups:

- /cbio/users
- /cbio/projects
- /cbio/soft
- /ilifu/users
- /ilifu/software
- Exception for ilifu projects:
  - /ilifu/astro/projects
  - /ilifu/bio/projects

ilifu

Directory Structure - Typical workflow

IDIA



*/n/data generally read-only

ilifu

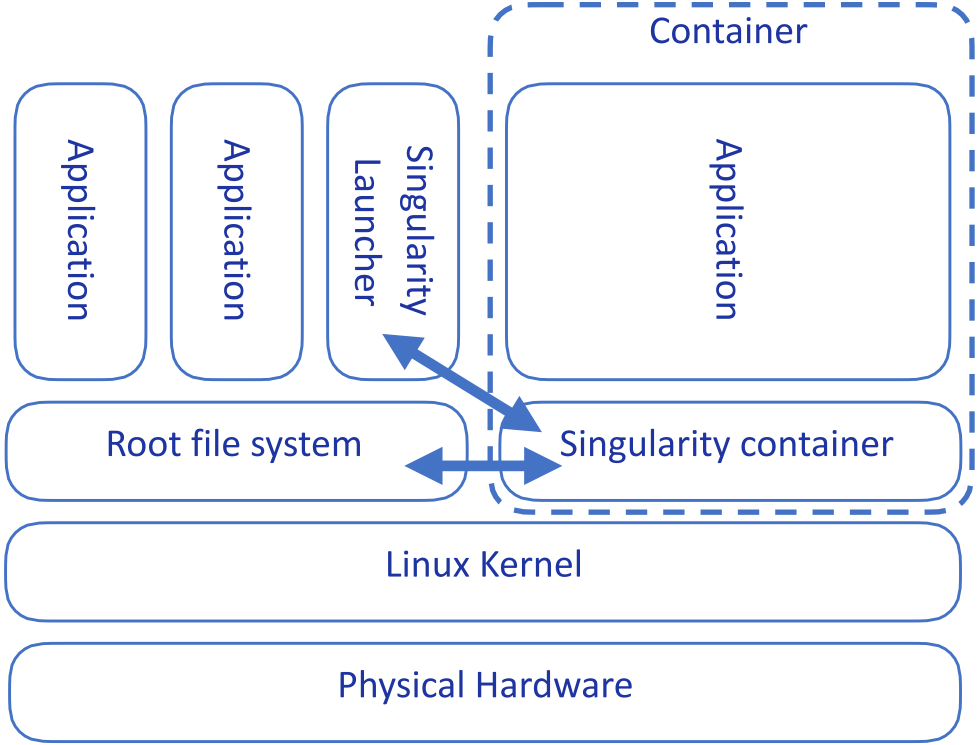
Software environment - Singularity containers

IDIA

- Encapsulated software environments
- A software stack that contains everything required to run an application/workflow, including files, environments variables, libraries and dependencies
- Containers accessible across platforms and services, allowing sharing of applications environments

https://sylabs.io/singularity

Software environment - Singularity containers



Software environment - Singularity containers

Supported Containers:

- CASA 5, CASA 6
- Astronomy container (ASTRO-PY3, ASTRO-PY3.8)
- KERN suite
- GPU Python container
- Project containers:
  - MeerLICHT, LADUMA, HI Intensity mapping
- lots of others

Directories:

- /software
- /idia/software/containers
- /ilifu/software/containers

Software environment - Singularity containers

Open container as an interactive shell:

```
singularity shell /path/to/container

Example:

$ singularity shell /idia/software/containers/ASTRO-PY3.8.simg
```

Run a script/workflow using a container environment:

```
singularity exec /path/to/container <software> <script/input_parameters>

$ singularity exec /idia/software/containers/casa-6.simg python myscript.py
```

Software environment - modules

module avail

```
$ module avail

----------------------------------------------------------------- /software/modules/common ------------------------------------------------------------------
   LAPACK/3.9.0                    anaconda3/2020.07              githubcli/2.0.0            mono/6.8.0.123        perlbrew/perlbrew    python/3.10.0
   R/RStudio1.2.5042-R4.0.0        anaconda3/2021.05              go/1.16.3                  mpich/3.3a2           python/2.7.18        python/3.10.1     (D)
   R/RStudio1.2.5042-R4.0.4        anaconda3/2021.11       (D)    go/1.17.3           (D)    openBLAS/0.3.9        python/3.6.15        ruby/2.6.6
   R/3.6.3                         cuda/10.0.130_410.48           graphviz/2.49.1            openmpi/2.1.1         python/3.7.7         singularity/2.6.1
   R/4.0.0                         cuda/10.1.243_418.87.00        homebrew/2.4.13            openmpi/2.1.6         python/3.8.2         singularity/3.7.3
   R/4.0.2                         cuda/10.2.89_440.33.01         hwloc/1.11.13              openmpi/3.1.6         python/3.8.3         singularity/3.8.3
   R/4.0.3                         cuda/11.0.2_450.51.05          java/jre-1.8.0_261         openmpi/4.0.3         python/3.8.6         singularity/3.9.0
   R/4.1.1                  (D)    cuda/11.4.2_470.57.02   (D)    java/openjdk-14.0.1 (D)    openmpi/4.0.5         python/3.9.0         singularity/3.9.1 (L,D)
   anaconda3/login.old             dotnet/5.0.301                 julia/1.5.3                openmpi/4.1.0  (D)    python/3.9.4         user_tools
   anaconda3/login                 drmaa/1.1.1                    maven/3.6.3                perl/5.33.0           python/3.9.7

------------------------------------------------------------------ /software/modules/astro ------------------------------------------------------------------
   casa/5.7.0      casa/5.8.0                   casa/6.1.2.7-pipeline    casa/6.2    casa/6.4     (D)
   casa/5.7.2-4    casa/6.1.0-118-monolithic    casa/6.1.2.7-modular     casa/6.3    pybdsf/1.9.2

------------------------------------------------------------------- /software/modules/bio -------------------------------------------------------------------
   bcbio/bcbio_container           biobambam2/2.0.183    genomestrip/2.00.1958    plink/2.00a2.3     samtools/1.13         vep/singularity
   bcbio/1.2.3                     canvas/1.40.0.1613    htslib/1.10.2            popgen/0.1         samtools/1.14   (D)   vep/101.0        (D)
   bcbio/1.2.9          (D)        cd-hit/4.8.2          mafft/7.490              prsice-2/2.3.1d    treePL/homebrew
   bcftools/1.10.2                 gemini/gemini         mash/2.3                 samtools/1.10      vcftools/0.1.16

------------------------------------------------------------- /usr/share/lmod/lmod/modulefiles --------------------------------------------------------------
   Core/lmod/6.6    Core/settarg/6.6

  Where:
   L:  Module is loaded
   D:  Default Module
```

ilifu

IDIA

Software environment - modules

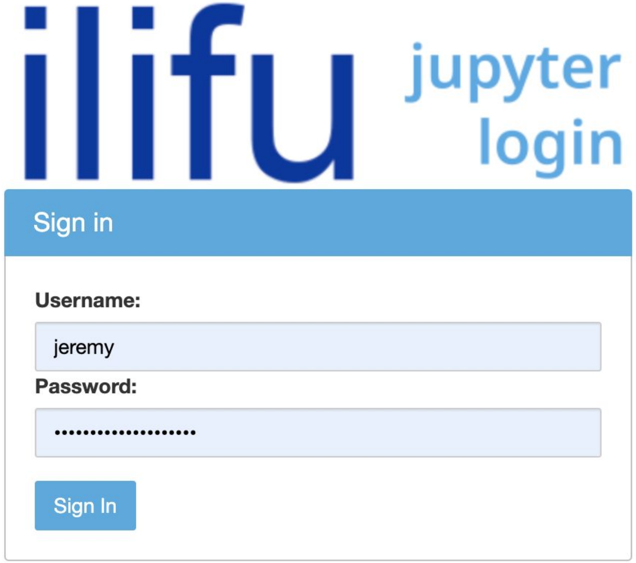
- module avail
- module help <module>

```
$ module help python

-------------------------------- Module Specific Help for "python/3.10.1" ---------------------------------
This module configures Python 3.10.1 for use
```

- module load <module>
- module list
- module purge
- module --help

JupyterHub

https://jupyter.ilifu.ac.za

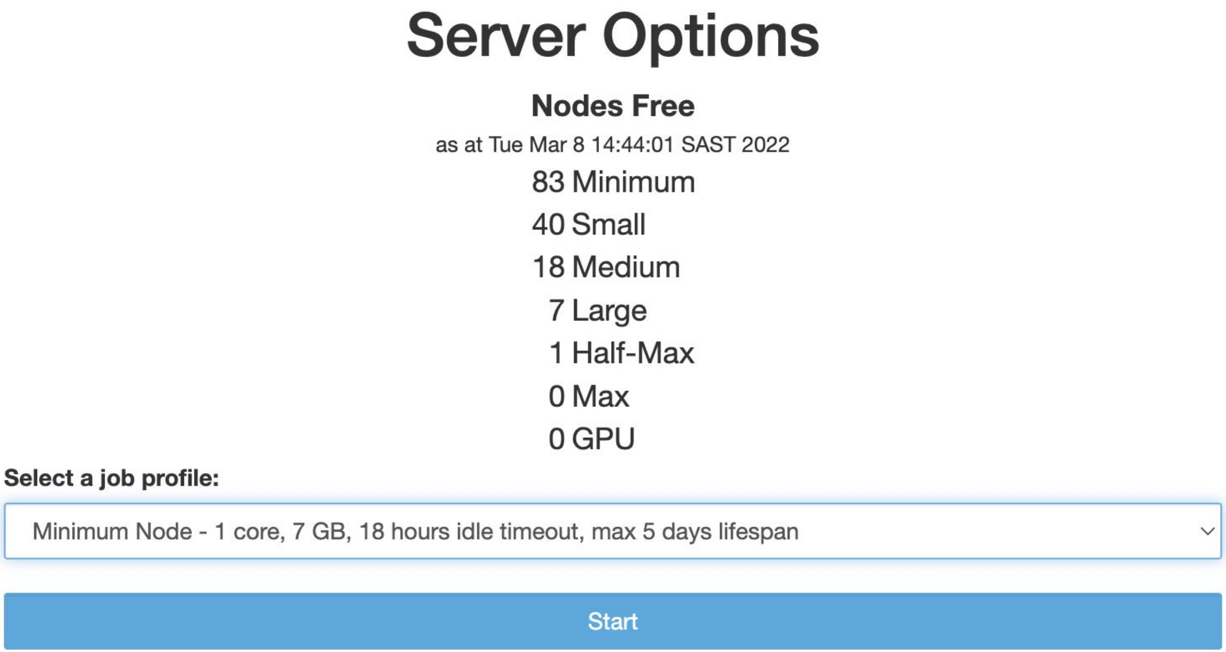


Username: jeremy

Password: ••••••••••••••••••••

JupyterHub

Session size



Server Options

Nodes Free

as at Tue Mar 8 14:44:01 SAST 2022

83 Minimum
40 Small
18 Medium
7 Large
1 Half-Max
0 Max
0 GPU

Select a job profile:

Minimum Node - 1 core, 7 GB, 18 hours idle timeout, max 5 days lifespan

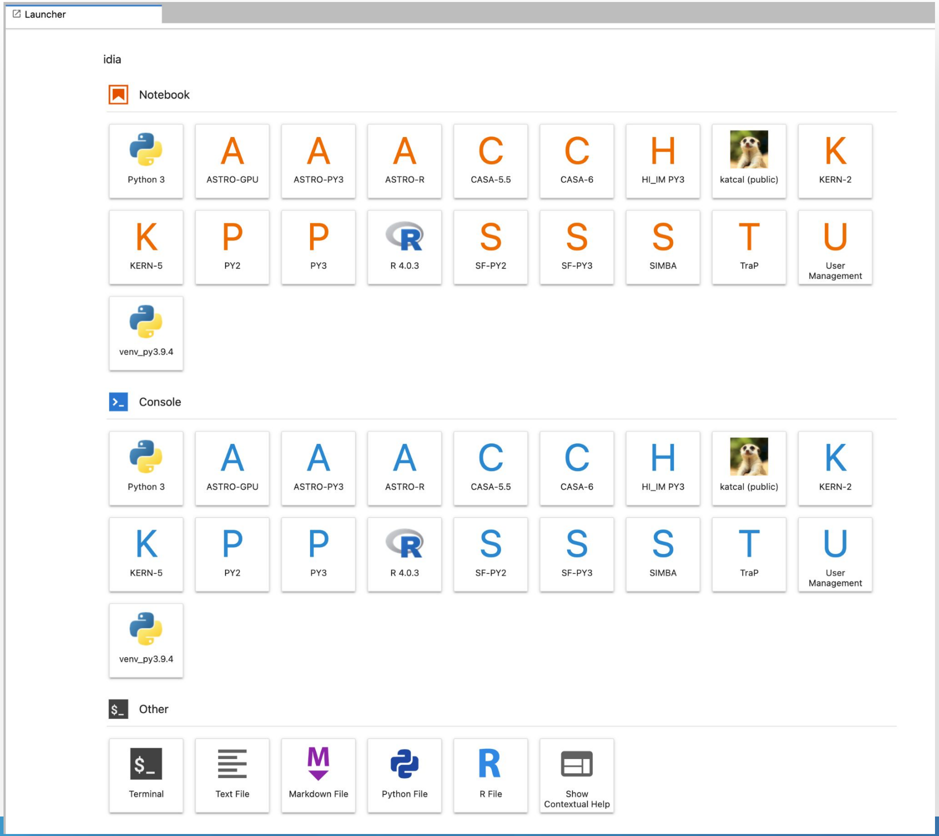
ilifu

IDIA

JupyterHub

Choose kernel

in launcher



Launcher

idia

Notebook

Python 3 | ASTRO-GPU | ASTRO-PY3 | ASTRO-R | CASA-5.5 | CASA-6 | HI_IM PY3 | katcal (public) | KERN-2 | KERN-5 | PY2 | PY3 | R 4.0.3 | SF-PY2 | SF-PY3 | SIMBA | TraP | User Management | venv_py3.9.4

Console

Python 3 | ASTRO-GPU | ASTRO-PY3 | ASTRO-R | CASA-5.5 | CASA-6 | HI_IM PY3 | katcal (public) | KERN-2 | KERN-5 | PY2 | PY3 | R 4.0.3 | SF-PY2 | SF-PY3 | SIMBA | TraP | User Management | venv_py3.9.4

Other

Terminal | Text File | Markdown File | Python File | R File | Show Contextual Help

ilifu

Demo

Demo resources https://github.com/ilifu/ilifu_user_training