IDIA Inter-University Institute for Data Intensive Astronomy

Ilifu Online Training

Session 1: Introduction to ilifu

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University of Cape Town · iYunivesithi yaseKapa · Universiteit van Kaapstad

University of the Western Cape

NRF National Research Foundation

SARAO South African Radio Astronomy Observatory

Topics

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

Getting help

- Support contact

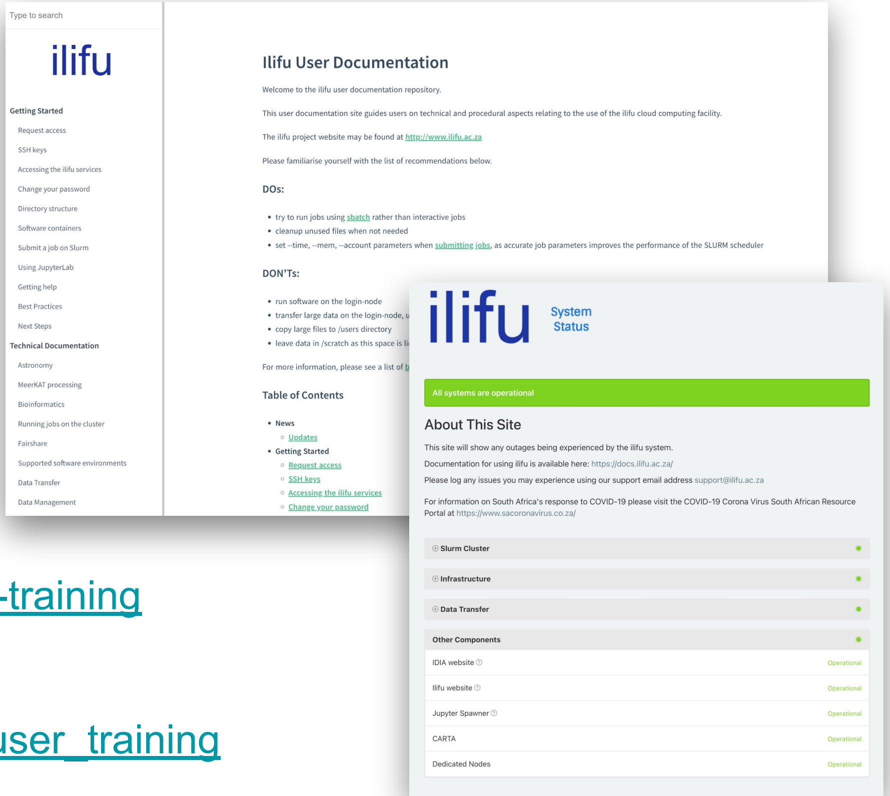
  support@ilifu.ac.za
- User documentation

  http://docs.ilifu.ac.za
- Ilifu System Status

  https://status.ilifu.ac.za
- Training videos

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

  https://github.com/ilifu/ilifu_user_training



Type to search

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
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- Getting Started
  - Request access
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  - Accessing the ilifu services
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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

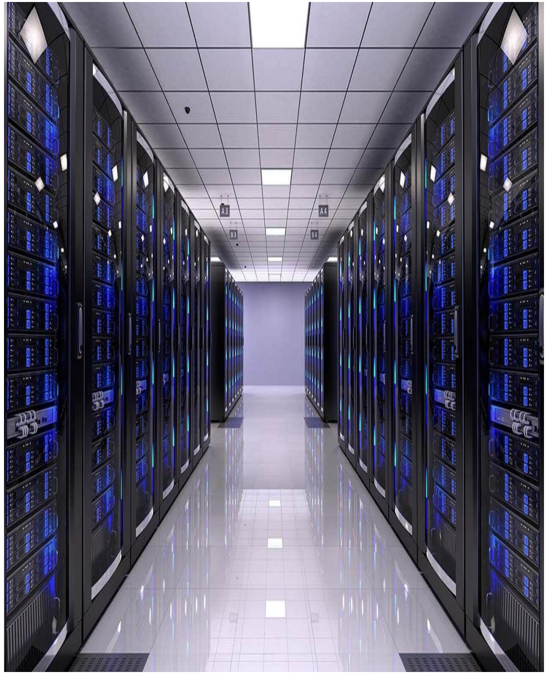
High Performance Computing

Combining power of compute clusters

- collection of servers (computers)
- connected by fast local network
- to solve complex problems

Some terminology

- computer system/server also referred to as a node
- group of nodes is a cluster



ilifu Research Facility

Cloud-based infrastructure for data-intensive research

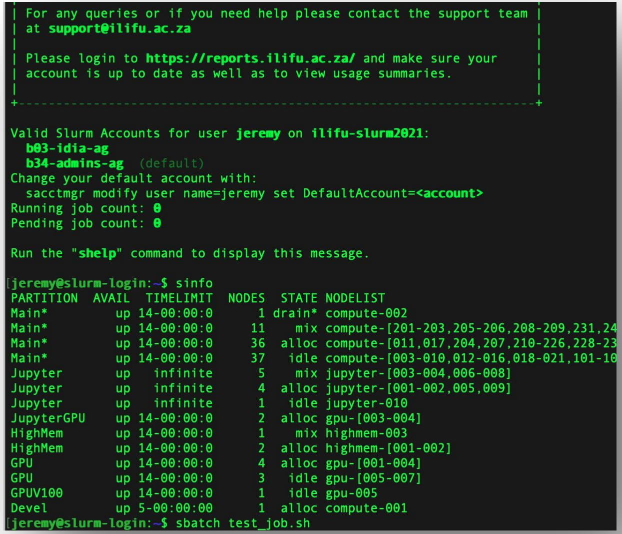
Network of remote servers, accessed over the internet, to store, manage, and process data

- Open source cloud software to deploy infrastructure as a service (IaaS)
- Support variety of different scientific projects and requirements
- Flexible compute environment
    - Cluster environment with workload management, additional services
- Data management: storage, transfer

ilifu Research Facility - interfaces

Command line interface

ssh - shell terminal



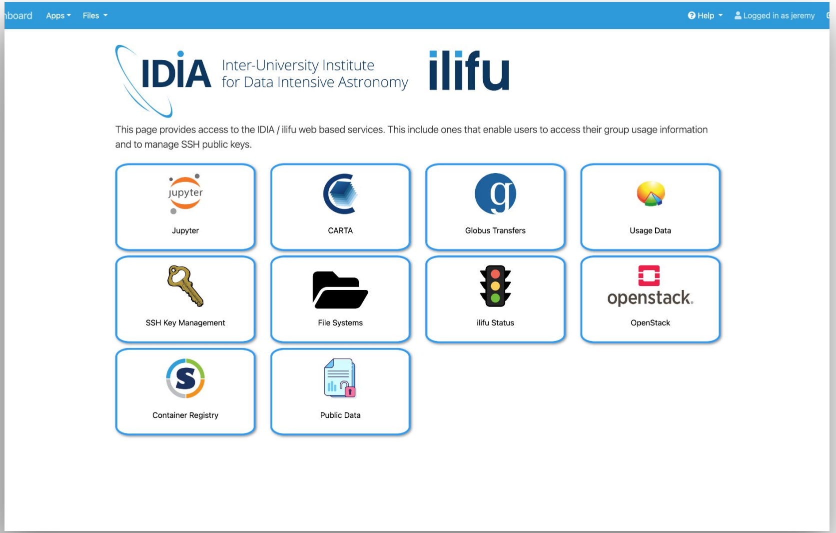
```
| For any queries or if you need help please contact the support team |
| at support@ilifu.ac.za                                              |
|                                                                     |
| Please login to https://reports.ilifu.ac.za/ and make sure your     |
| account is up to date as well as to view usage summaries.           |
|                                                                     |
+---------------------------------------------------------------------+

Valid Slurm Accounts for user jeremy on ilifu-slurm2021:
  b03-idia-ag
  b34-admins-ag  (default)
Change your default account with:
  sacctmgr modify user name=jeremy set DefaultAccount=<account>
Running job count: 0
Pending job count: 0

Run the "shelp" command to display this message.

[jeremy@slurm-login:~$ sinfo
PARTITION  AVAIL  TIMELIMIT  NODES  STATE NODELIST
Main*         up 14-00:00:0      1 drain* compute-002
Main*         up 14-00:00:0     11    mix compute-[201-203,205-206,208-209,231,24
Main*         up 14-00:00:0     36  alloc compute-[011,017,204,207,210-226,228-23
Main*         up 14-00:00:0     37   idle compute-[003-010,012-016,018-021,101-10
Jupyter       up   infinite      5    mix jupyter-[003-004,006-008]
Jupyter       up   infinite      4  alloc jupyter-[001-002,005,009]
Jupyter       up   infinite      1   idle jupyter-010
JupyterGPU    up 14-00:00:0      2  alloc gpu-[003-004]
HighMem       up 14-00:00:0      1    mix highmem-003
HighMem       up 14-00:00:0      2  alloc highmem-[001-002]
GPU           up 14-00:00:0      4  alloc gpu-[001-004]
GPU           up 14-00:00:0      3   idle gpu-[005-007]
GPUV100       up 14-00:00:0      1   idle gpu-005
Devel         up 5-00:00:00      1  alloc compute-001
[jeremy@slurm-login:~$ sbatch test_job.sh
```

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

`ssh <username>@transfer.ilifu.ac.za`

Web applications

IDIA Science Gateway - App Dashboard



This page provides access to the IDIA / ilifu web based services. This include ones that enable users to access their group usage information and to manage SSH public keys.

https://gateway.idia.ac.za

ilifu Research Facility - Web Applications

Application dashboard - accessed via https://gateway.idia.ac.za

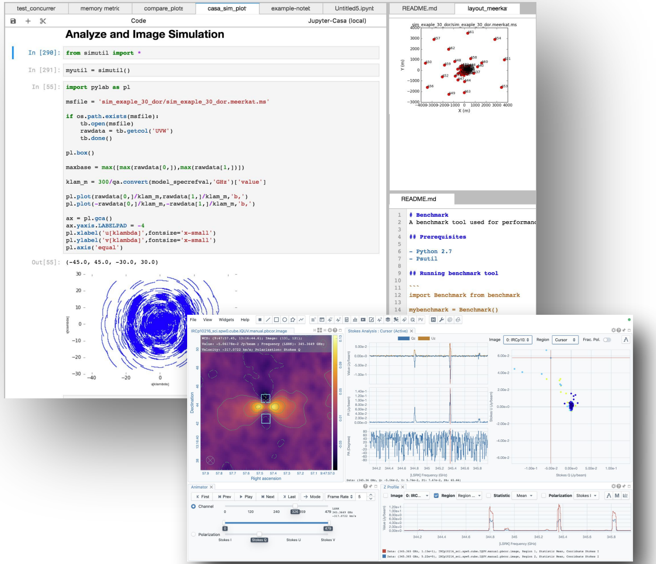
Welcome to the IDIA Science Gateway. This provides access to IDIA resources. For information about IDIA see www.idia.ac.za.

Access secure IDIA / ilifu resources. An ilifu account is required for this. This will give you access to various resources including Jupyter Notebooks, CARTA, SSH Key Management, Globus and OpenStack. This also allows you to link your institution account to your ilifu account using eduGAIN / SAFIRE.

Request an ilifu account for access to the IDIA / ilifu systems.

IDIA provides access to public data sets that can be accessed without an IDIA account.

This page provides access to the IDIA / ilifu web based services. This include ones that enable users to access their group usage information and to manage SSH public keys.



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()
```

Web application examples

https://jupyter.ilifu.ac.za

https://carta.idia.ac.za
```

Compute 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
- Default:
  - ~/.ssh/id_rsa ~/.ssh/id_rsa.pub
  - ~/.ssh/id_ed25519 ~/.ssh/id_ed25519.pub

Compute environment - ssh

Generating SSH key

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

Manage your SSH keys associated with your ilifu account

https://usage.ilifu.ac.za/ssh_keys

Compute environment - ssh

```
user-local:~$ ssh <username>@slurm.ilifu.ac.za
...
<username>@slurm-login:~$
<username>@slurm-login:~$ pwd
/users/<username>
<username>@slurm-login:~$ ls
README.md  workspace
<username>@slurm-login:~$ ls /idia/projects/
G4Jy          gamma-ray-binaries  meerlicht           shapley-uhf
M64-NGC151    goodsn              meerlirgs           share
adfs          grandspiral         meerrings           simba
antlia        hack4dev            merghers            supermightee
...
```

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. **Limited to 200GB**
- /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. **Limited to 10TB**
- /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

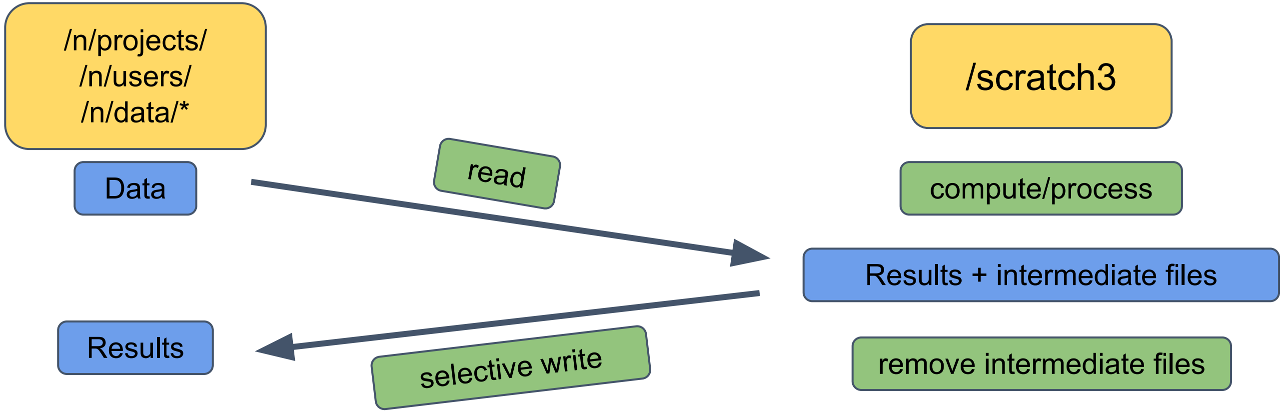
Similar structure for /cbio and /ilifu groups:

- /cbio/users **(Limited to 10TB)**
- /cbio/projects
- /cbio/soft
- /ilifu/users **(Limited to 2TB)**
- /ilifu/software
- Exception for ilifu projects:
    - /ilifu/astro/projects
    - /ilifu/bio/projects

Directory Structure - Typical workflow

/users

Scripts and small files only



/n/projects/
/n/users/
/n/data/*

Data

read

/scratch3

compute/process

Results + intermediate files

selective write

Results

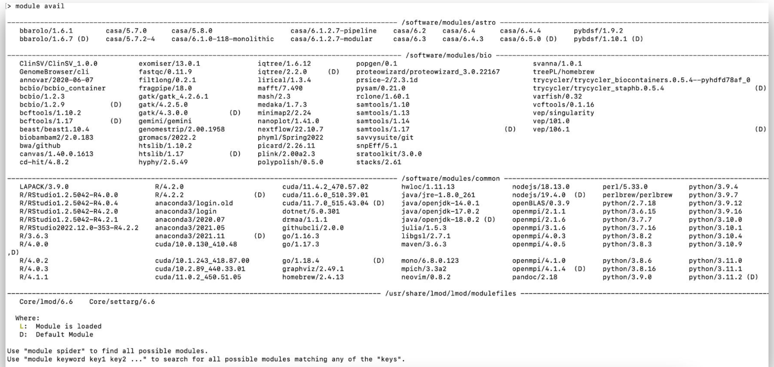
remove intermediate files

*/n/data generally read-only

n = idia,cbio,ilifu

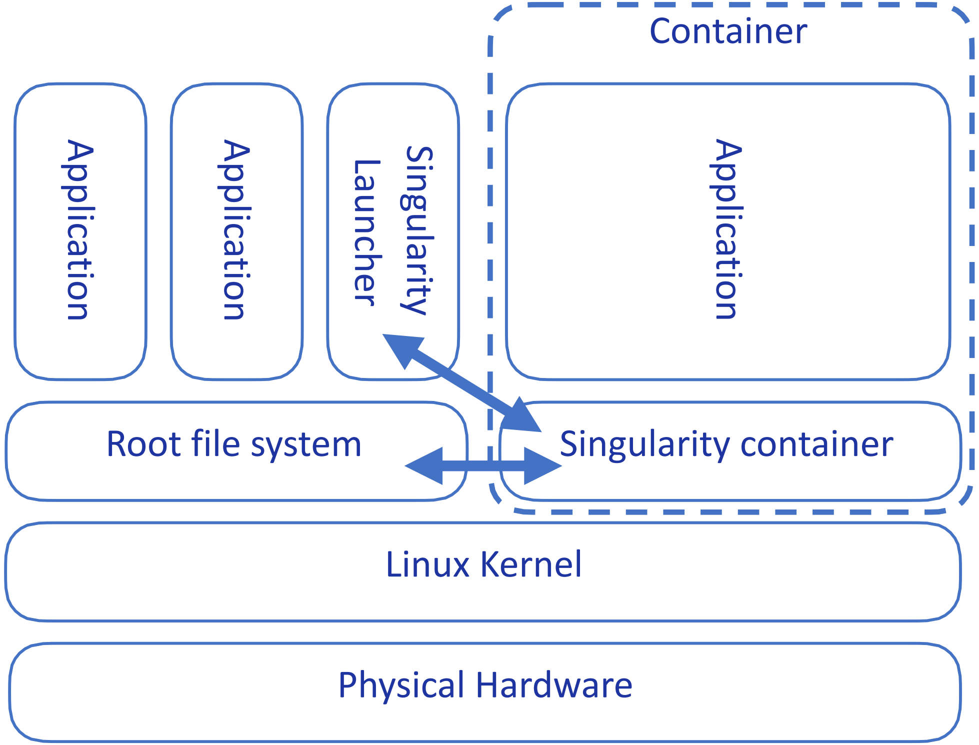
Ilifu Software Environment

- Software containers
  - encapsulated software environments
  - suite of applications and libraries
  - shareable, transferable to different hardware/environments
  - reproducible science
- Modules
  - common languages & utilities (CUDA, MPI)
  - ease of use
  - wrapper for containers
- Virtual environments
  - Python, conda
  - user created & managed
  - useful for prototyping & development



```
> module avail

--------------------------------------------------------------------------------------- /software/modules/astro ------------------------------------------------------------
   bbarolo/1.6.1        casa/5.7.0      casa/5.8.0                     casa/6.1.2.7-pipeline    casa/6.2    casa/6.4      casa/6.4.4        pybdsf/1.9.2
   bbarolo/1.6.7 (D)    casa/5.7.2-4    casa/6.1.0-118-monolithic      casa/6.1.2.7-modular     casa/6.3    casa/6.4.3    casa/6.5.0 (D)    pybdsf/1.10.1 (D)

---------------------------------------------------------------------------------------- /software/modules/bio -------------------------------------------------------------
   ClinSV/ClinSV_1.0.0               exomiser/13.0.1                  iqtree/1.6.12            popgen/0.1                                     svanna/1.0.1
   GenomeBrowser/cli                 fastqc/0.11.9                    iqtree/2.2.0      (D)    proteowizard/proteowizard_3.0.22167            treePL/homebrew
   annovar/2020-06-07                filtlong/0.2.1                   lirical/1.3.4            prsice-2/2.3.1d                                trycycler/trycycler_biocontainers.0.5.4--pyhdfd78af_0
   bcbio/bcbio_container             fragpipe/18.0                    mafft/7.490              pysam/0.21.0                                   trycycler/trycycler_staphb.0.5.4                      (D)
   bcbio/1.2.3                       gatk/gatk_4.2.6.1                mash/2.3                 rclone/1.60.1                                  varfish/0.32
   bcbio/1.2.9                (D)    gatk/4.2.5.0                     medaka/1.7.3             samtools/1.10                                  vcftools/0.1.16
   bcftools/1.10.2                   gatk/4.3.0.0              (D)    minimap2/2.24            samtools/1.13                                  vep/singularity
   bcftools/1.17              (D)    gemini/gemini                    nanoplot/1.41.0          samtools/1.14                                  vep/101.0
   beast/beast1.10.4                 genomestrip/2.00.1958            nextflow/22.10.7         samtools/1.17                           (D)    vep/106.1                                             (D)
   biobambam2/2.0.183                gromacs/2022.2                   phyml/Spring2022         savvysuite/git
   bwa/github                        htslib/1.10.2                    picard/2.26.11           snpEff/5.1
   canvas/1.40.0.1613                htslib/1.17               (D)    plink/2.00a2.3           sratoolkit/3.0.0
   cd-hit/4.8.2                      hyphy/2.5.49                     polypolish/0.5.0         stacks/2.61

--------------------------------------------------------------------------------------- /software/modules/common -----------------------------------------------------------
   LAPACK/3.9.0                        R/4.2.0                              cuda/11.4.2_470.57.02         hwloc/1.11.13                nodejs/18.13.0        perl/5.33.0           python/3.9.4
   R/RStudio1.2.5042-R4.0.0            R/4.2.2                       (D)    cuda/11.6.0_510.39.01         java/jre-1.8.0_261           nodejs/19.4.0  (D)    perlbrew/perlbrew     python/3.9.7
   R/RStudio1.2.5042-R4.0.4            anaconda3/login.old                  cuda/11.7.0_515.43.04 (D)     java/openjdk-14.0.1          openBLAS/0.3.9        python/2.7.18         python/3.9.12
   R/RStudio1.2.5042-R4.2.0            anaconda3/login                      dotnet/5.0.301                java/openjdk-17.0.2          openmpi/2.1.1         python/3.6.15         python/3.9.16
   R/RStudio1.2.5042-R4.2.1            anaconda3/2020.07                    drmaa/1.1.1                   java/openjdk-18.0.2 (D)      openmpi/2.1.6         python/3.7.7          python/3.10.0
   R/RStudio2022.12.0-353-R4.2.2       anaconda3/2021.05                    githubcli/2.0.0               julia/1.5.3                  openmpi/3.1.6         python/3.7.16         python/3.10.1
   R/3.6.3                             anaconda3/2021.11             (D)    go/1.16.3                     libgsl/2.7.1                 openmpi/4.0.3         python/3.8.2          python/3.10.4
   R/4.0.0                             cuda/10.0.130_410.48                 go/1.17.3                     maven/3.6.3                  openmpi/4.0.5         python/3.8.3          python/3.10.9
,D)
   R/4.0.2                             cuda/10.1.243_418.87.00              go/1.18.4              (D)    mono/6.8.0.123               openmpi/4.1.0         python/3.8.6          python/3.11.0
   R/4.0.3                             cuda/10.2.89_440.33.01               graphviz/2.49.1               mpich/3.3a2                  openmpi/4.1.4  (D)    python/3.8.16         python/3.11.1
   R/4.1.1                             cuda/11.0.2_450.51.05                homebrew/2.4.13               neovim/0.8.2                 pandoc/2.18           python/3.9.0          python/3.11.2 (D)

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

  Where:
   L:  Module is loaded
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

Software environment - Singularity containers



Software environment - Singularity containers

Supported Containers:

- CASA 5, CASA 6
- Astronomy container (ASTRO-PY3, ASTRO-PY3.8, ASTRO-PY3.10)
- 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-PY3.10.sif
```

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
```

Look at what is inside a container by viewing its build script:

```
singularity inspect -d /path/to/container

$ singularity inspect -d /idia/software/containers/casa-6.simg
```

Software environment - modules

module avail

```
$ module avail

----------------------------------------------------------------------- /software/modules/astro -----------------------------------------------------------------------
   atnfcat/2.0.1        casa/5.7.2-4                 casa/6.2      casa/6.5.0           cfitsio/4.3.1   (D)    pybdsf/1.9.2           splinter/a968918
   bbarolo/1.6.1        casa/5.8.0                   casa/6.3      casa/6.5.5           pgplot/5.2             pybdsf/1.10.1   (D)    tempo/0b487e2
   bbarolo/1.6.7 (D)    casa/6.1.0-118-monolithic    casa/6.4      casa/6.6.0           psrcat/1.50            qd/2.3.12              tempo2/2024.02.1
   calceph/2.3.2        casa/6.1.2.7-pipeline        casa/6.4.3    casa/6.6.4    (D)    psrdada/008afa7        sigproc/28ba4f4
   casa/5.7.0           casa/6.1.2.7-modular         casa/6.4.4    cfitsio/3.450        psrxml/1.01            sofa/20180130

------------------------------------------------------------------------ /software/modules/bio ------------------------------------------------------------------------
   ClinSV/ClinSV_1.0.0          filtlong/0.2.1               merqury/1.3                                samtools/1.18
   DIANN/1.8.1                  fragpipe/18.0                meryl/1.3                                  samtools/1.19
   GenomeBrowser/cli            gatk/gatk_4.2.6.1            meryl/1.4.1                         (D)    samtools/1.19.2
   ambertools/23                gatk/4.2.5.0                 minimap2/2.24                              samtools/1.20                                         (D)
   annovar/2020-06-07           gatk/4.3.0.0                 miniwdl/1.12.1                             savvysuite/git
   bamtools/2.5.2               gatk/4.4.0.0                 mtoolbox/1.2.1.1                           seqkit/2.6.0
   bcbio/bcbio_container        gatk/4.5.0.0          (D)    multiqc/1.17                               seqtk/1.4
   bcbio/1.2.3                  gemini/gemini                multiqc/1.22.3                      (D)    seqwish/0.7.9-2
   bcbio/1.2.9           (D)    gemma/0.98.5                 mummer/4.0.0rc1                            shapeit5/5.1.1
   bcftools/1.10.2              genomestrip/2.00.1958        nanocomp/1.23.1                            snpEff/5.1
   bcftools/1.17                gfastats/1.3.6               nanofilt/2.8.0                             snpdists/0.8.2
   bcftools/1.19         (D)    glimpse/2.0.0                nanoplot/1.41.0                            snpsites/2.5.1
 ...
---------------------------------------------------------------------- /software/modules/common -----------------------------------------------------------------------
   LAPACK/3.9.0                         cuda/11.0.2_450.51.05          gnuplot/default            neovim/0.8.2             python/3.9.7
   LAPACK/3.10.1                        cuda/11.4.2_470.57.02          go/1.16.3                  neovim/0.9.4      (D)    python/3.9.12
   LAPACK/3.12.0                 (D)    cuda/11.6.0_510.39.01          go/1.17.3                  nodejs/18.13.0           python/3.9.16
   R/RStudio1.2.5042-R4.0.0             cuda/11.7.0_515.43.04          go/1.18.4                  nodejs/19.4.0     (D)    python/3.9.19
   R/RStudio1.2.5042-R4.0.4             cuda/11.8.0_520.61.05          go/1.20.4                  openBLAS/0.3.9           python/3.10.0
   R/RStudio1.2.5042-R4.2.0             cuda/12.1.0_530.30.02          go/1.21.6                  openBLAS/0.3.20          python/3.10.1
   R/RStudio1.2.5042-R4.2.1             cuda/12.2.0_535.54.03          go/1.22.4           (D)    openBLAS/0.3.25   (D)    python/3.10.4
   R/RStudio2022.12.0-353-R4.2.2        cuda/12.4.0_550.54.14   (D)    graphviz/2.49.1            openmpi/2.1.1            python/3.10.9
...
------------------------------------------------------------------- /opt/lmod/lmod/modulefiles/Core ------------------------------------------------------------------
   lmod    settarg

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

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
```

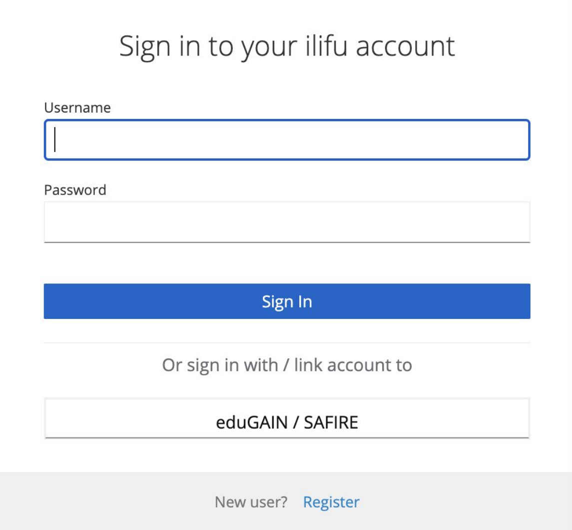
- module load <module>
- module list
- module purge
- module --help

JupyterHub

https://gateway.idia.ac.za

OR

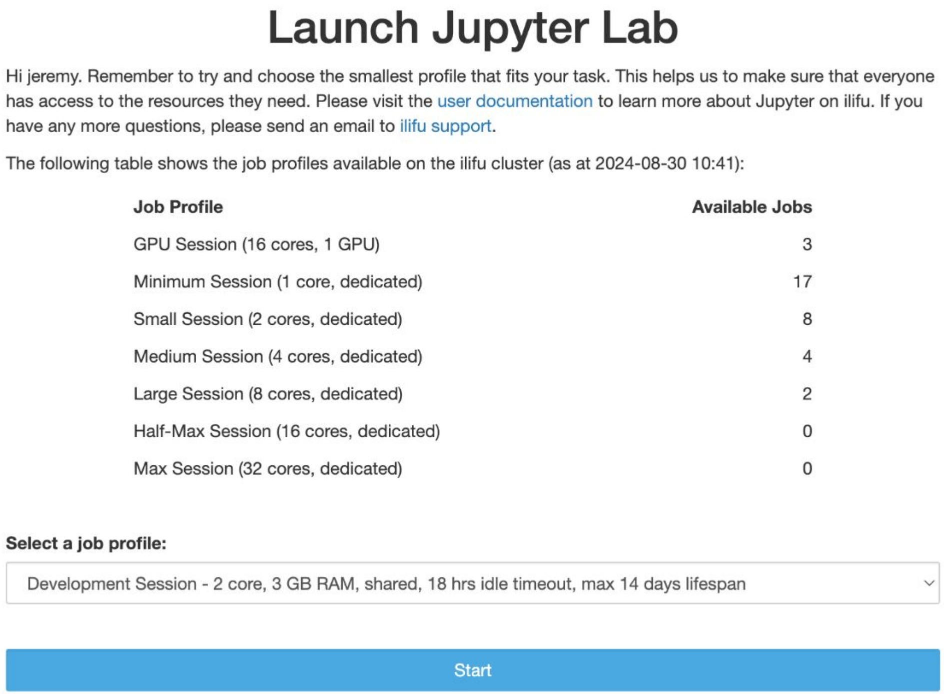
https://jupyter.ilifu.ac.za



This page provides access to the IDIA / ilifu web based services. This include ones that enable users to access their group usage information and to manage SSH public keys.

JupyterHub

Session size



Launch Jupyter Lab

Hi jeremy. Remember to try and choose the smallest profile that fits your task. This helps us to make sure that everyone has access to the resources they need. Please visit the user documentation to learn more about Jupyter on ilifu. If you have any more questions, please send an email to ilifu support.

The following table shows the job profiles available on the ilifu cluster (as at 2024-08-30 10:41):

Job Profile	Available Jobs
GPU Session (16 cores, 1 GPU)	3
Minimum Session (1 core, dedicated)	17
Small Session (2 cores, dedicated)	8
Medium Session (4 cores, dedicated)	4
Large Session (8 cores, dedicated)	2
Half-Max Session (16 cores, dedicated)	0
Max Session (32 cores, dedicated)	0

Select a job profile:

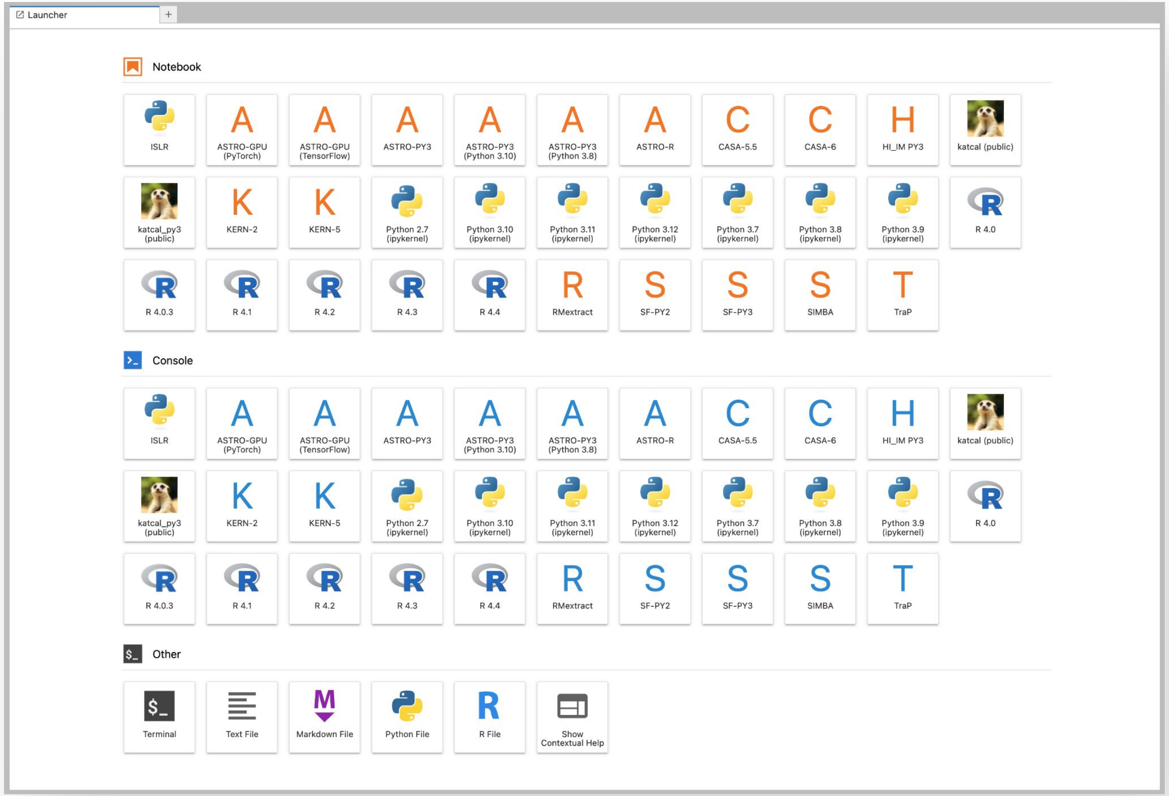
Development Session - 2 core, 3 GB RAM, shared, 18 hrs idle timeout, max 14 days lifespan

IDIA

JupyterHub

Choose kernel

in launcher



ilifu

Demo

Demo resources

- https://github.com/ilifu/ilifu_user_training