



IDiA Inter-University Institute for Data Intensive Astronomy

Ilifu Online Training

Session 2: Software environments

9 September 2025

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Topics

- Software environments
 - Python virtual environments
 - Using R and RStudio
- Advanced Slurm usage
 - Interactive jobs in Slurm
 - Advanced Slurm commands

Getting help

- Support contact

support@ilifu.ac.za

- User documentation

<http://docs.ilifu.ac.za>

- Ilifu System Status

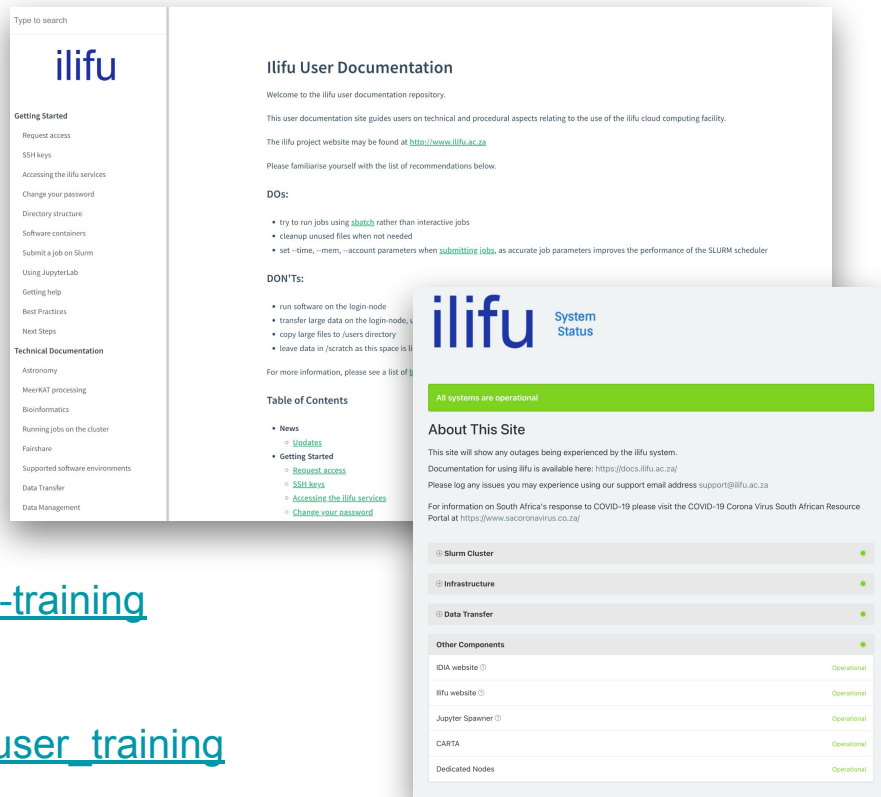
<https://status.ilifu.ac.za>

- Training videos

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

- Training tutorials

https://github.com/ilifu/ilifu_user_training



The image displays three overlapping screenshots of the ilifu website. The top-left screenshot shows the 'ilifu' homepage with a sidebar menu containing links like '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', 'MixeKAT processing', 'Bioinformatics', 'Running jobs on the cluster', 'Fairshare', 'Supported software environments', 'Data Transfer', and 'Data Management'. The top-right screenshot shows the 'ilifu User Documentation' page, which includes a welcome message, a link to the project website, and a list of recommendations for users. The bottom-right screenshot shows the 'ilifu System Status' page, which features a green banner stating 'All systems are operational' and a table listing the status of various components.

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 [slurbs](#) 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, i
- copy large files to /users directory
- leave data in /scratch as this space is li

For more information, please see a list of g

Table of Contents

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- Getting Started
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 - [SSH keys](#)
 - [Accessing the ilifu services](#)
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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/>

Component	Status
Slurm Cluster	Operational
Infrastructure	Operational
Data Transfer	Operational
Other Components	
IDIA website	Operational
ilifu website	Operational
Jupyter Spawner	Operational
CARTA	Operational
Dedicated Nodes	Operational

Python Virtual Environments

virtualenv

- Availability anywhere
- <https://virtualenv.pypa.io/en/latest/>
- Isolated Python environment
- Less risk of conflicts occurring with `pip install --user`
- Similar to `venv` (`python -m venv`)
- Can customize which os python is used: `python2.7`, `python3+`
- Installable packages limited by os libraries

Python Virtual Environments

```
module load python/3.12.3*
```

```
virtualenv --help
```

```
virtualenv /path/to/virtual_environment
```

```
--python The Python interpreter to use
```

```
--system-site-packages Gives the virtual environment  
access to the global  
site-packages
```

* Use a module to create a virtual environment, rather than system Python, as a change to the OS can break venvs created with the system Python.

Python Virtual Environments

Create a new Python virtual environment:

```
virtualenv /path/to/virtual/environment
```

Example:

```
$ virtualenv venv/tutenv
```

```
$ source venv/tutenv/bin/activate           #to enter
```

```
(tutenv)$ which python
```

```
    /.../venv/tutenv/bin/python
```

```
(tutenv)$ python -m pip install scikit-learn
```

```
(tutenv)$ deactivate                       #to exit
```

Python Virtual Environments

Python virtualenv as a Jupyter kernel

Once the virtual environment is active:

```
python -m pip install ipykernel  
ipython kernel install --name "<kernel_name>" --user
```

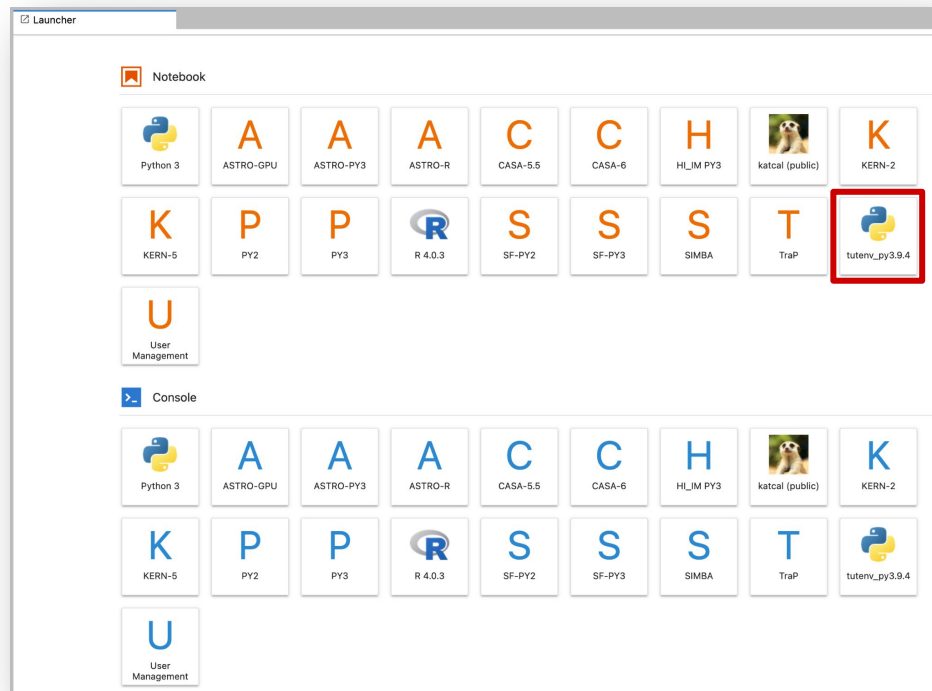
Example:

```
source venv/tutenv/bin/activate  
python -m pip install ipykernel  
ipython kernel install --name "tutenv_py3.9.4" --user  
Installed kernelspec jupyter in ~/.local/share/jupyter/kernels/tutenv_py3.9.4
```

Creates the kernel.json file at:

```
~/.local/share/jupyter/kernels/tutenv_py3.9.4/kernel.json
```

Python Virtual Environments



R and RStudio with slurm

https://docs.ilifu.ac.za/#/tech_docs/software_environments?id=running-rstudio-server

When logged in via ssh:

```
jeremy@slurm-login:~$ srun --nodes=1 --tasks=1 --mem=8g --time
08:00:00 --job-name="rstudio test" --pty bash
```

```
jeremy@compute-001:~$ module add R/RStudio2023.06.1-524-R4.4.1
```

```
jeremy@compute-001:~$ rstudio
```

The environment variable RSTUDIO_PASSWORD was not set, so your password has been chosen for you. It's: *****

Running rserver on port 40739

To connect to this server run this on your local machine:

```
ssh -A jeremy@compute-001 -o "ProxyCommand=ssh
jeremy@slurm.ilifu.ac.za nc compute-001 22" -L8081:localhost:40739
```

then visit <http://localhost:8081> in your browser and use the username "jeremy" to login with the password "*****"

(You may need to choose a different port (other than 8081), so remember to change this in both the ssh and browser)

R and Studio with slurm

https://docs.ilifu.ac.za/#/tech_docs/software_environments?id=running-r-studio-server

On your local machine:

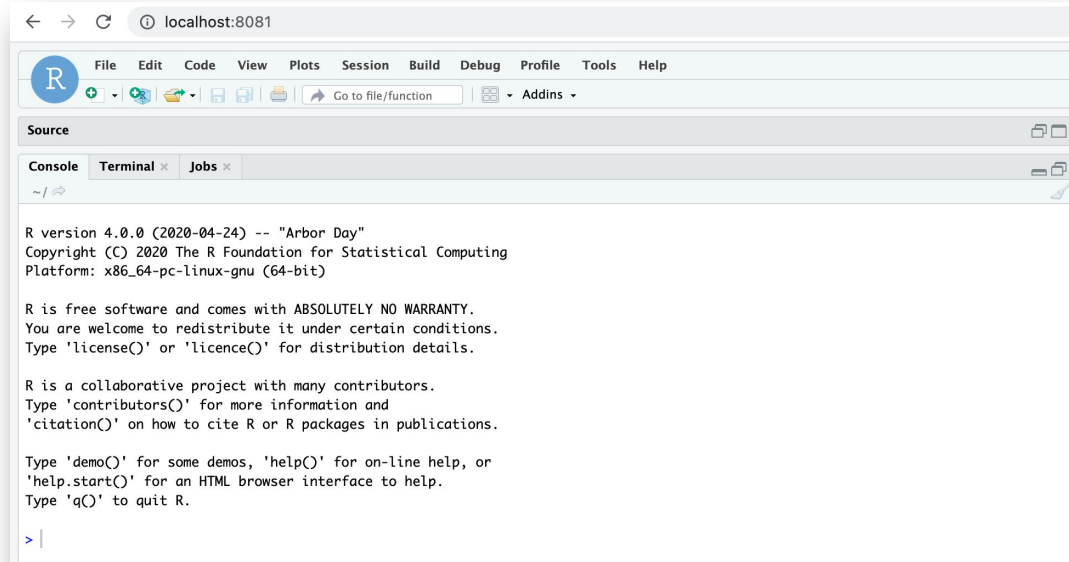
```
jeremy:~$ ssh -A jeremy@compute-001 -o "ProxyCommand=ssh  
jeremy@slurm.ilifu.ac.za nc compute-001 22" -L8081:localhost:40739
```

Go to: <http://localhost:8081> in your local browser

R and Studio with slurm

https://docs.ilifu.ac.za/#/tech_docs/software_environments?id=running-r-studio-server

Now you can access RStudio through you web browser:



Software Environment summary

virtual environment

- Good for prototyping and rapid development
- User created and managed
- Can be used by a group but needs to be in appropriate folder
- Limited by available os libraries

Modules

- Variety of languages, bioinformatics and utility software
- Useful for software that doesn't have a lot of dependencies
- Some modules execute containers more conveniently

Containers

- Best for reproducibility and sharing
- Best for software that requires libraries/dependencies
- Can be used by anyone with the path



Collections

[New Collection](#) [Labels](#) [Rankings](#) [Topic Tags](#)

Top Collections All Collections

Name	Builds	Private	Modified
casa	26 [cases, 'casa-modular', 'casa-modular-ev310', 'casa-stable', 'casa-rb-rcorgd']	No	2024-08-16
calibration	16 [calibagger, 'offset', 'silfman', 'hycon', 'silvay44', 'sens2-silfman', 'writing_book', 'traf', 'silfman', 'oskar', 'booklet', 'tom-carmer', 'si', 'samoy', 'vscs44']	No	2024-08-16
ev3hon	24 [astro-ev3, 'astro-ev310', 'astro-mc81']	No	2024-05-08
spica	11 [spica]	No	2024-05-08

Private	Modified
No	2024-08-16
No	2024-08-16
No	2024-05-08
No	2024-05-08
No	2024-05-08
No	2024-05-14
No	2024-05-15

A screenshot of the IDIA (Interactive Data Infrastructure Assistant) interface. A modal dialog box titled "casa/casa:v6.4.3" is open, displaying instructions for using Singularity. The dialog contains three sections: "Singularity Examples" with a link to a user guide, "Pull the container:" with commands for pulling the container from a library or registry, "Shell into the container:" with commands for opening a shell, and "Run the container:" with commands for running the container. The background shows a table of installed containers with columns for name, version, and dates.