



IDI*A*

Inter-University Institute
for Data Intensive Astronomy

Ilifu Online Training

Session 2: Software environments

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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

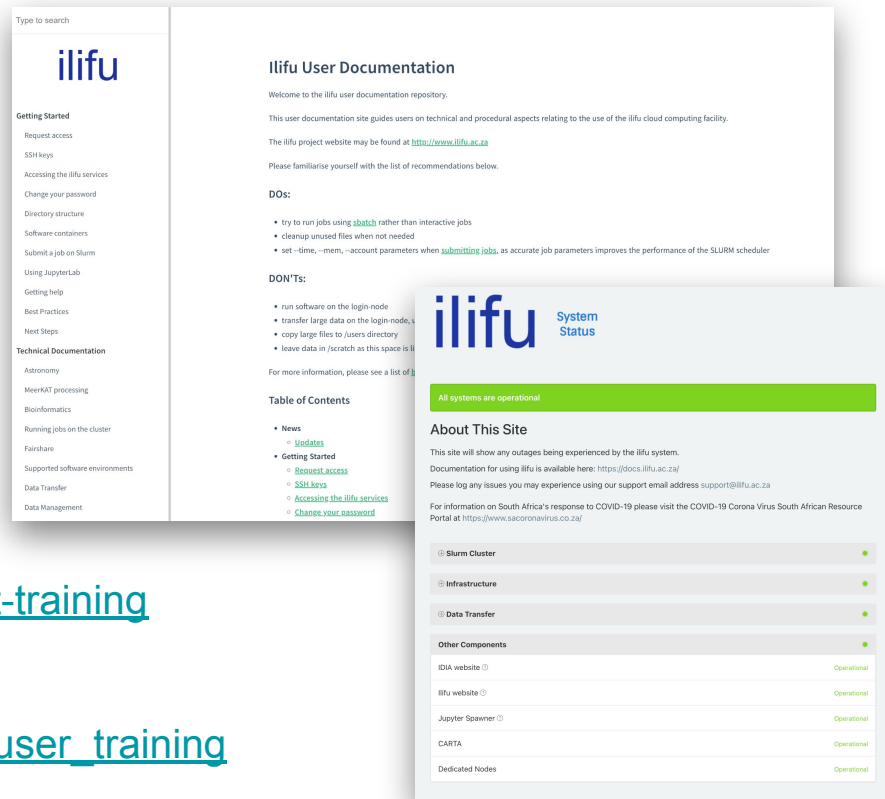
<https://status.ilifu.ac.za>

- Training videos

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

- Training tutorials

https://github.com/ilifu/ilifu_user_training



The image shows three overlapping screenshots of the ilifu website. The top-left screenshot is the 'ilifu' user documentation repository page, featuring a search bar, a navigation menu with categories like 'Getting Started', 'Technical Documentation', and 'Astronomy', and a main content area with 'ilifu User Documentation' and a 'Table of Contents'. The top-right screenshot is the 'ilifu System Status' page, which has a green banner stating 'All systems are operational' and a table listing system components like 'Slurm Cluster', 'Infrastructure', and 'Data Transfer', all marked as operational. The bottom screenshot is a detailed view of the 'System Status' page, showing a table of components with their status: IDIA website (Operational), ilifu website (Operational), Jupyter Spawner (Operational), CARTA (Operational), and 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
```

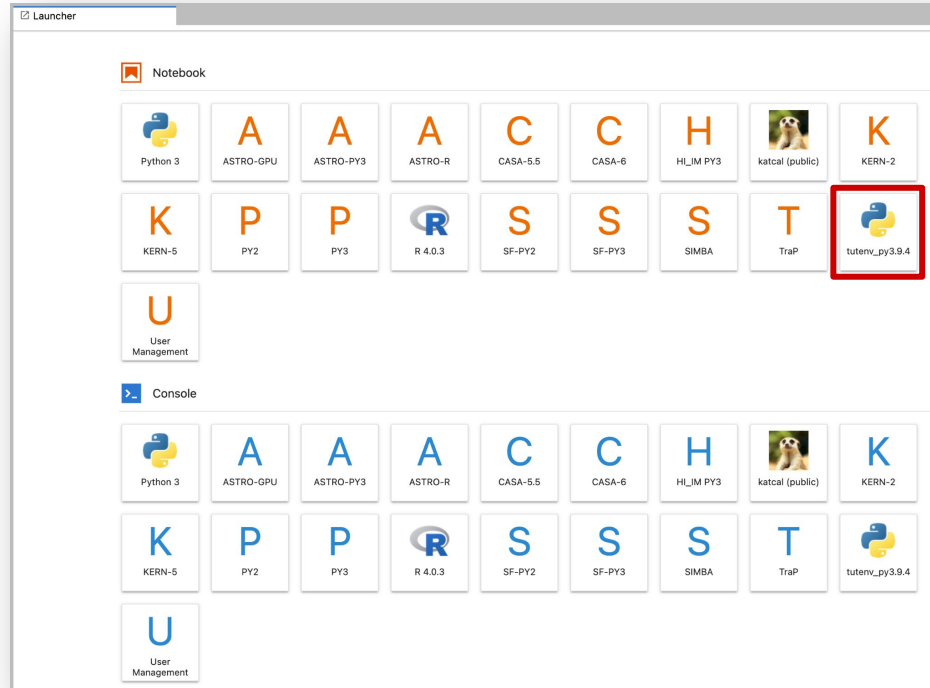
Example:

```
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:

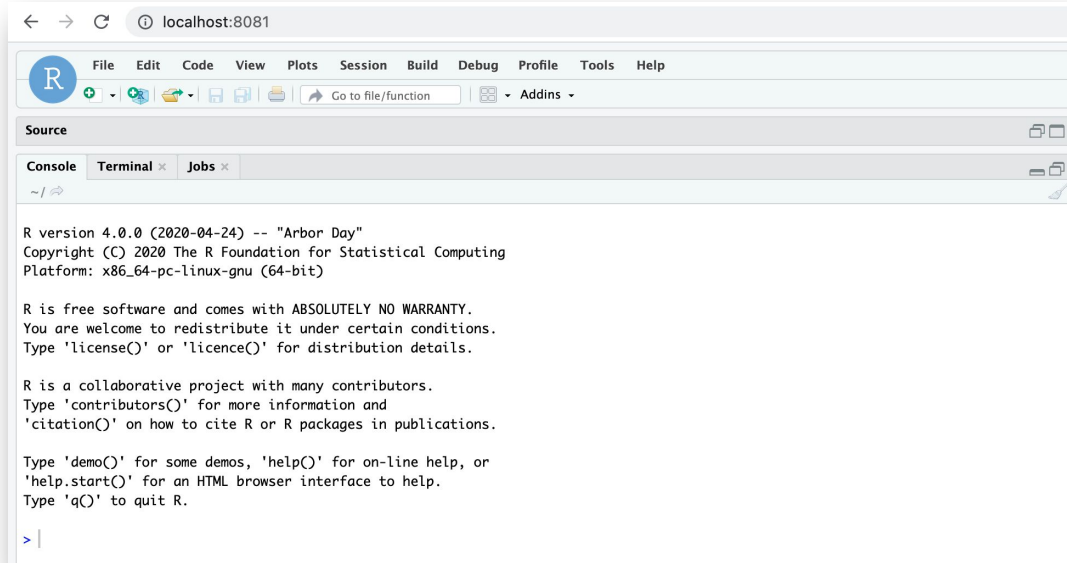
```
jeremy:~$ ssh -A jeremy@compute-001 -o "ProxyCommand=ssh  
jeremy@slurm.ilifu.ac.za nc compute-001 22" -L8081:localhost:40739
```

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:



```
localhost:8081
R
File Edit Code View Plots Session Build Debug Profile Tools Help
Source
Console Terminal x Jobs x
~/
R version 4.0.0 (2020-04-24) -- "Arbor Day"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> |
```

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