ilifu Online Training

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User Training Workshop – Advanced Training #1
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Topics

- Software environment
  - Python virtual environments
  - Using R and RStudio
- Advanced Slurm usage
  - Advanced Slurm commands
  - Interactive sessions in Slurm
- Data transfers

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/

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+
- Limited by os libraries

Python Virtual Environments

```
virtualenv --help

virtualenv
/path/to/virtual_environment

--python

--system-site-packages
```

The Python interpreter to user

Gives the virtual environment access to the global site-packages

Python Virtual Environments

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

Example:

```
virtualenv ~/.venv/tutenv
source ~/.venv/tutenv/bin/activate
(tutenv) jeremy@compute-060:~$ which python
   ~/.venv/tutenv/bin/python
pip install scikit-learn
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
```

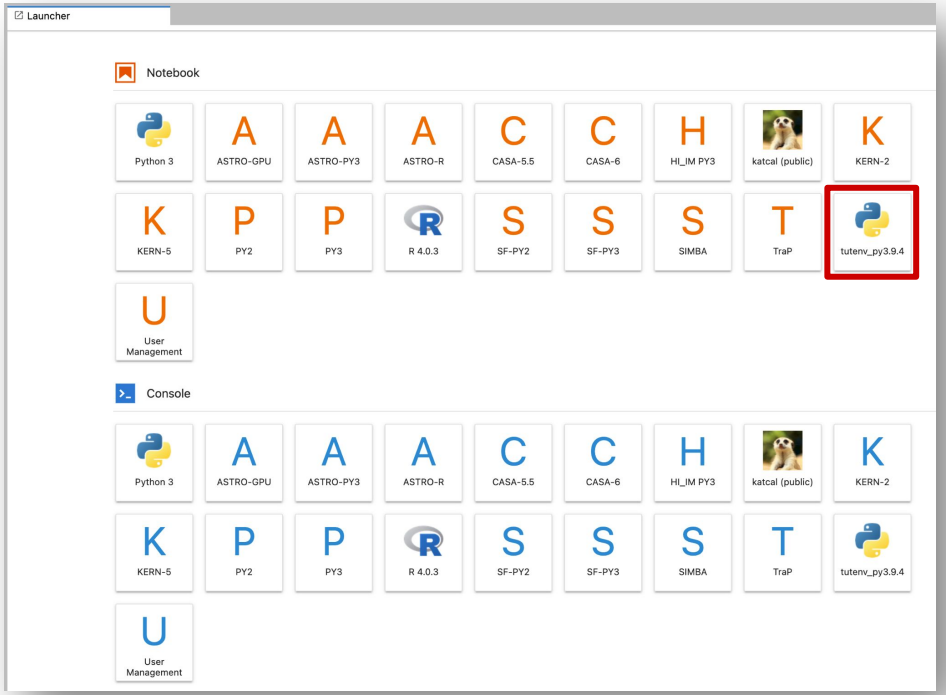
Example:

```
source ~/.venv/tutenv/bin/activate

python -m pip install ipykernel

ipython kernel install --name "tutenv_py3.9.4" --user

Installed kernelspec jupkernel 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/RStudio1.2.5042-R4.0.0

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-rstudio-server

On your local machine:

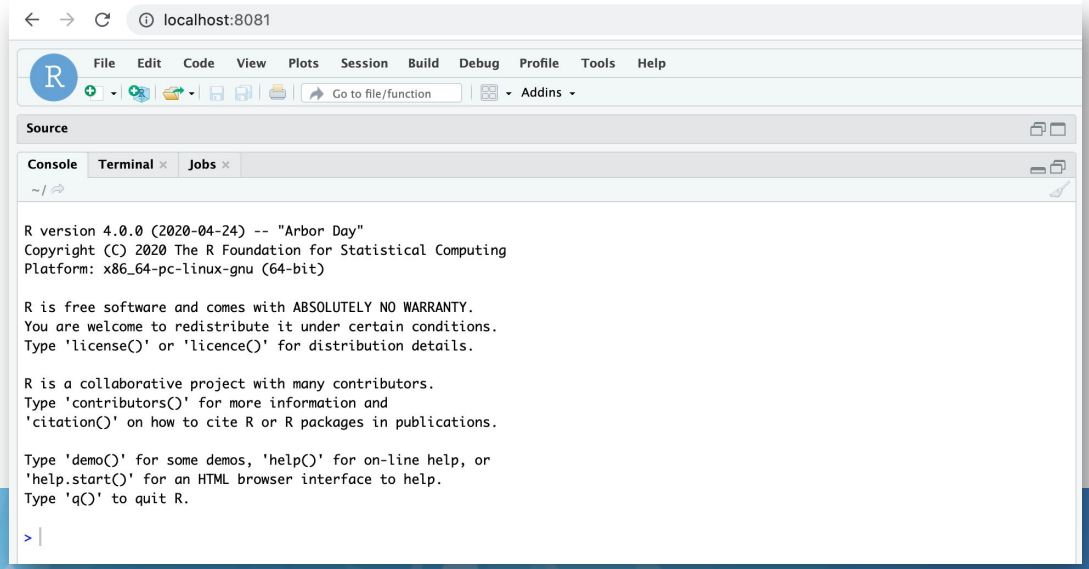
```
jeremy:~$ ssh -A jeremy@compute-001 -o "ProxyCommand=ssh
jeremy@slurm.ilifu.ac.za nc compute-001 22" -L8081:localhost:40739
```

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-rstudio-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

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