ilifu Online Training

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User Training Workshop – Advanced Training

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Topics

- Python virtual environments
- R and RStudio
- Building Singularity containers

Python Virtual Environments

virtualenv

- Available 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`	*The Python interpreter to use*
`--system-site-packages`	*Give the virtual environment access to the global site-packages*

Python Virtual Environments

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

Example:

```
virtualenv ~/.jupenv
source ~/.jupenv/bin/activate
(.jupenv) robh@slurm-login:~$
which python
    ~/.jupenv/bin/bin/python
pip install scikit-learn
deactivate (to exit)
```

Python Virtual Environments

Python virtualenv as a Jupyter kernel

Once the virtual environment is active:

```
ipython kernel install --name ”<kernel_name>" --user
```

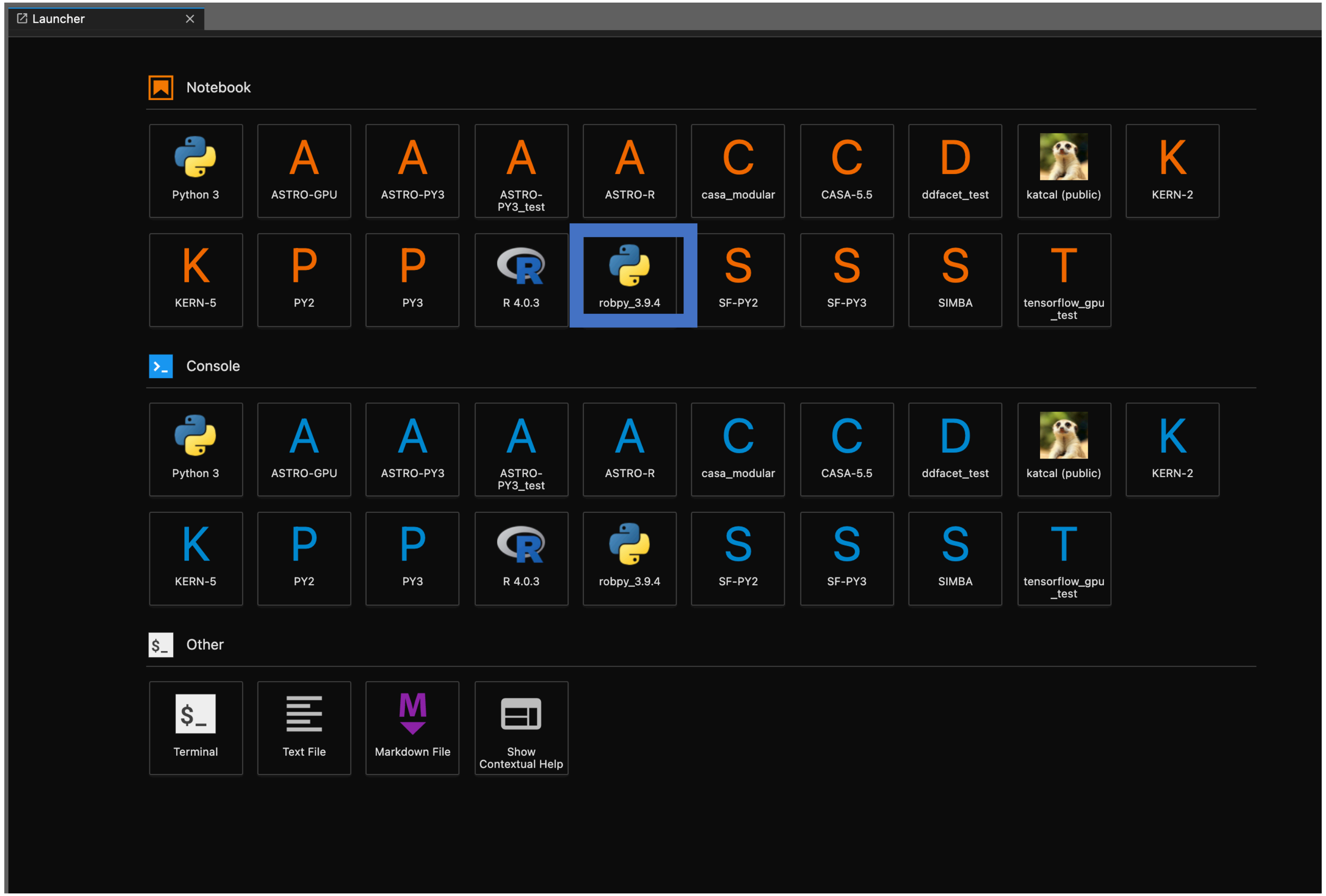
Example:

```
source ~/.jupenv/bin/activate
pip install jupyter
ipython kernel install --name "robpy_3.9.4" --user
Installed kernelspec robpy_3.9.4 in /users/robh/.local/share/
jupyter/kernels/robpy_3.9.4
```

Creates the kernel.json file at:

```
/users/robh/.local/share/jupyter/kernels/robpy_3.9.4/kernel.json
```

Python Virtual Environments



R and RStudio with slurm

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

When logged in via ssh:

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

robh@compute-004:~$ module add R/RStudio1.2.5042-R4.0.0

robh@compute-004:~$ rstudio
The environment variable RSTUDIO_PASSWORD was not set, so your
password has been chosen for you. It's: ******
Running rserver on port 40755
To connect to this server run this on your local machine:
       ssh -A robh@compute-004 -o "ProxyCommand=ssh
       robh@slurm.ilifu.ac.za nc compute-004 22"
       -L8081:localhost:40755
then vist http://localhost:8081 in your browser and use the username
"robh" to login with the password ******
```

R and Studio with slurm

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

On your local machine:

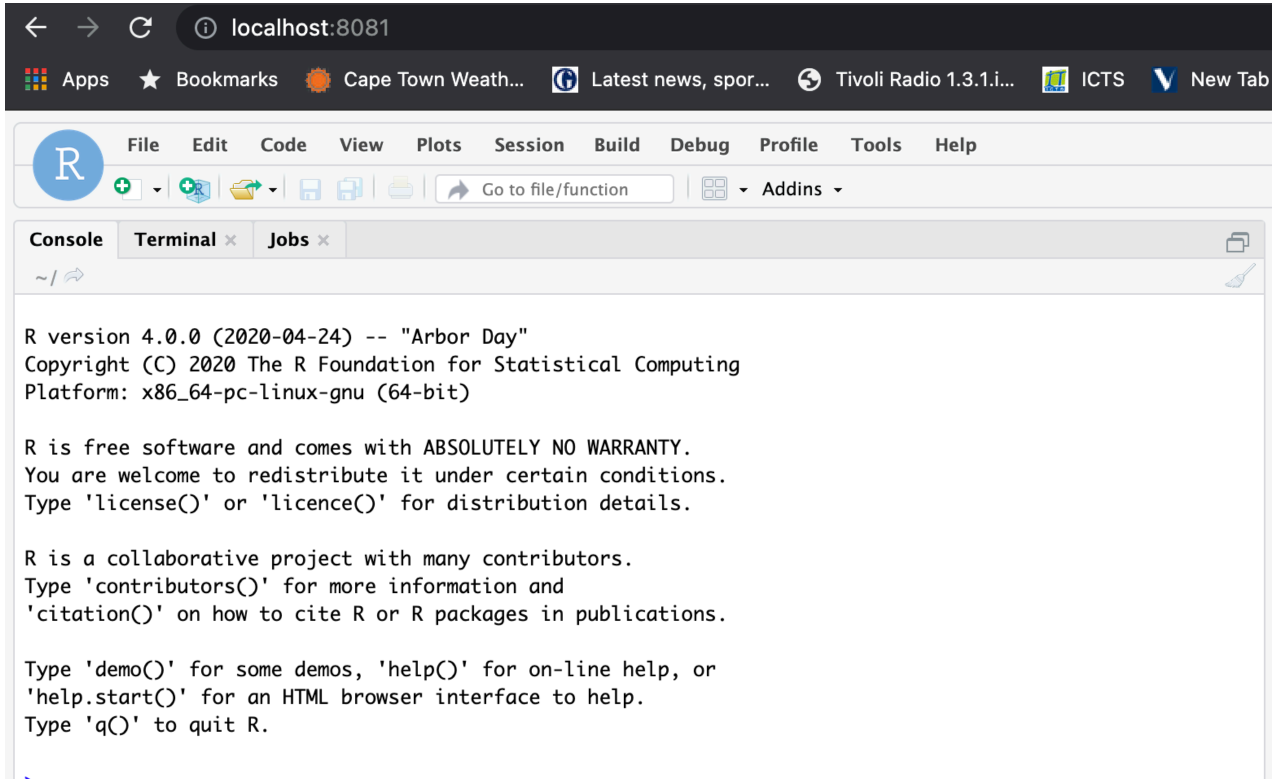
```
robinh@MacBook-Pro[~] -> % ssh -A robh@compute-004 -o
"ProxyCommand=ssh robh@slurm.ilifu.ac.za nc
compute-004 22" -L8081:localhost:40755
```

Go to: http://localhost:8081

R and Studio with slurm

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

Now you can access RStudio through your web browser:



```
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.
```

Singularity containers

Singularity 3.0 definition files

https://sylabs.io/guides/3.0/user-guide/definition_files.html

Singularity containers

```
Bootstrap: docker
From: ubuntu:18.04

%files
    /file1
    /file1 /opt

%environment
    export LISTEN_PORT=12345
    export PYTHONPATH=training_demo/:$PYTHONPATH

%post
    apt update
    apt-get install -y python3 python3-pip git

%runscript
    python3 "$@"
```

Header:

- base OS
- Keywords depend on selection

Singularity containers

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```

Files:

- Copy files from host to container
- Source and destination

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Environment:

- Variables set at runtime

Singularity containers

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Post:

- Commands to build on OS
- Customise container

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    apt update
    apt-get install -y python3 python3-pip git

%runscript
    python3 "$@"
```

Runscript:

- Executed when container is run

Singularity containers

Build container:

```
sudo singularity build <definition_file.def>
<container_name.simg>
```

Run container:

```
singularity run <container_name.simg> <args>

singularity exec <container_name.simg> <args>

singularity shell <container_name.simg>
```

Demo time

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IDIA

Summary of Software Environs.

virtual environment

- Good for prototyping and rapid development
- Can be used by a group but needs to be in appropriate folder

Module

- Useful if container doesn't have version of software
- Some modules execute containers more conveniently

Containers

- Best for reproducibility and sharing
- Can be used by anyone with the path