

Gadi Setup

Agenda in Meeting

- Brief points on q&a week 1 and 2.
- Demo how to start JupyterLab session.
- Finalize a python version for everyone to use.

Important

- I created `mq_venv`, a venv that **should be used by everyone**. Install libraries such as TensorFlow here. `Team` will need to `load python3/3.9.2` and `activate the venv` before starting the `JupyterLab session`.

Launch JupyterLab Session

1. SSH: `ssh -Y ky5750@gadi.nci.org.au` `UTAR43000Kajang$`
2. `cd /scratch/mq91`
3. Load python module: `module load python3/3.9.2` Check loaded module: `module list`
4. `source mq91_venv/bin/activate`
5. Install libraries if needed.
6. Login [are.nci.org.au](https://www.nci.org.au): `ky5750` `UTAR43000Kajang$`
7. Press JupyterLab, modify input if needed, press launch.

Interactive Apps

Desktops

VDI Desktop

VDI Desktop - GPU-enabled

Servers

JupyterLab

RStudio

RStudio (Rocker image)

JupyterLab version: 6e4fe1e

Launch a JupyterLab session

Walltime (hours)

1

Number of hours your jupyter session can run (maximum). e.g. 1.5, 8, 24, 48

Queue

normalbw

Compute Size

small

Amount of CPU/Memory resources available to your jupyter session

Project

mq91

Project to submit gadi job under; requires an SU allocation

Storage

scratch/mq91

Software

abaqus abaqus_rmit adf ansys_monash ansys_mq ansys_nci ansys_rmit

☒ I would like to receive an email when the session starts

Advanced options ...

SU estimate

2 cpu cores + 9GB mem on normalbw queue (1.25 SUs/core/h) for 1h = 2.5 SUs

Launch

* The JupyterLab session data for this session can be accessed under the [data root directory](#).

Extra arguments

Space-separated list of additional arguments to pass on the jupyterlab commandline

Module directories

Include module directories, eg **/g/data/hr22/modulefiles** (the equivalent of 'module use /g/data/hr22/modulefiles' on the command line). Make sure you add any **storage** option (above) required to access the directory (eg gdata/hr22 in this example)

Modules

python3/3.9.2

Space-separated list of modules to load, eg **julia/1.9.1 R/4.3.1** (the equivalent of 'module load julia/1.9.1 R/4.3.1' on the command line)

Python or Conda virtual environment base

/scratch/ma91/ma91 venv

Conda environment

Activates a specific conda environment within a conda install eg **myenv**. Requires the path to the conda base environment above (the equivalent of 'conda activate myenv' on the command line)

Environment variables

Space-separated list of environment variables to define (via pbs 'qsub -v') e.g. NAME="VALUE"

Jobfs size

The maximum amount of local disk available to the session. e.g. 10GB, 100MB

PBS flags

Define any extra pbs qsub flags.

Pre-script

A script / executable to run prior to starting app. Note: must have executable permission set

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Install libraries

1. cd `/scratch/mq91/mq91_venv/lib/python3.9/site-packages`.
2. `python3 -m pip install tensorflow`
3. Show installed libraries in the venv: `ls`

Other Commands

- Check quota: `lquota`
- Check snapshots (backups): `cd .snapshot` from root directory.
- Check for python3 modules available to install: `module avail python3*`
- Check for jobs running: `qstat`
- Available modules: `module avail`