



Introduction to Gadi

NCI Training

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Overview

- NCI: a collaboration of stakeholders representing Australian research community
- Gadi: NCI peak HPC system
- Get access to Gadi
- Showcase
 - Login
 - Basic application workflow
 - Submit and monitor jobs
 - Monitor project usage
 - Use applications installed on /apps
 - Build your own python/R/Julia packages on Gadi
 - Monitor job efficiency



NCI & Gadi

National Computational Infrastructure

What is NCI

- HPC for Australian researchers
 - 55 stakeholders, including universities, research institutes, and Australian Government agencies
 - 2600+ projects
 - 5500+ users
- Services
 - High performance computing
 - Data storage and services: THREDDS and VDI etc
 - Cloud computing





NCI & Gadi

Gadi: Australia's Peak Research Supercomputer

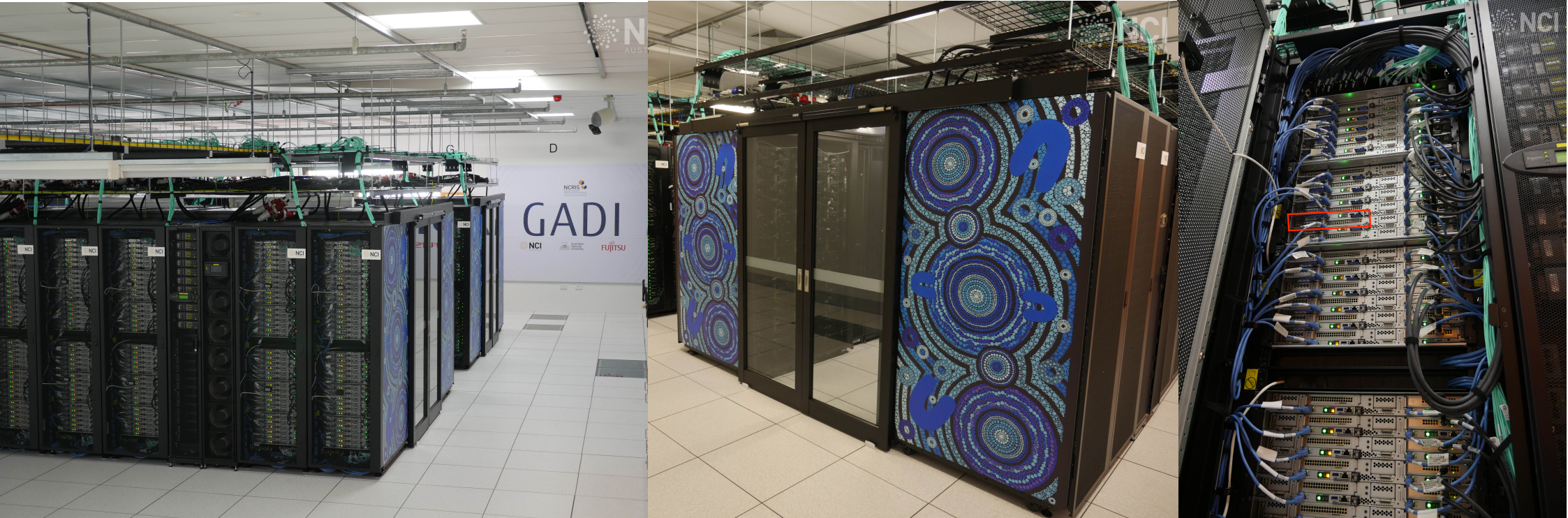
What is Gadi

- High performance computing system operated by NCI
- Pronounced `gar dee`, means `*to search for*` in the language of the Ngunnawal people
- Located on ANU Acton campus
- Launched in 2019 , replaced Raijin (2013-2020)
- In 2021 Q1, Gadi ran ~4M jobs for 1659 users from 650 projects

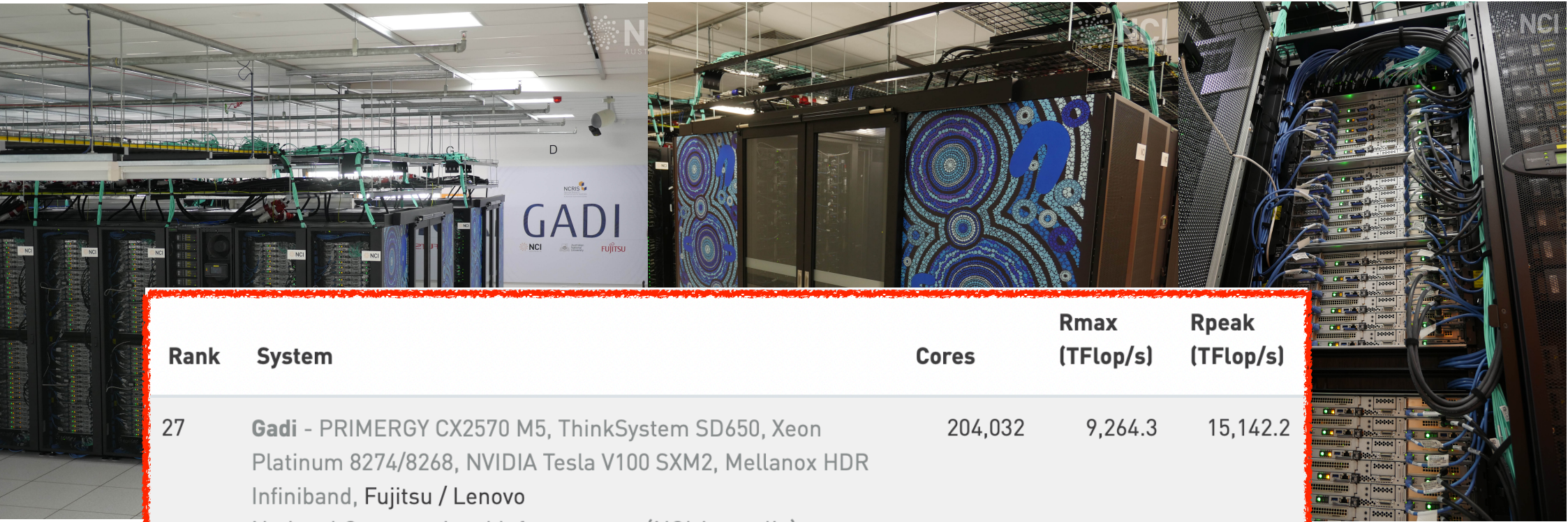
What is Gadi

- Supercomputer
 - 4000+ compute nodes, including 160 GPU nodes
 - 10 login nodes
 - 6 data mover nodes
 - PiB parallel file systems
 - Mellanox HDR InfiniBand interconnect network in Dragonfly+ topology
 - Application software catalogue
 - PBS Pro server 2021.1
 - CentOS 8.3.2011

Gadi

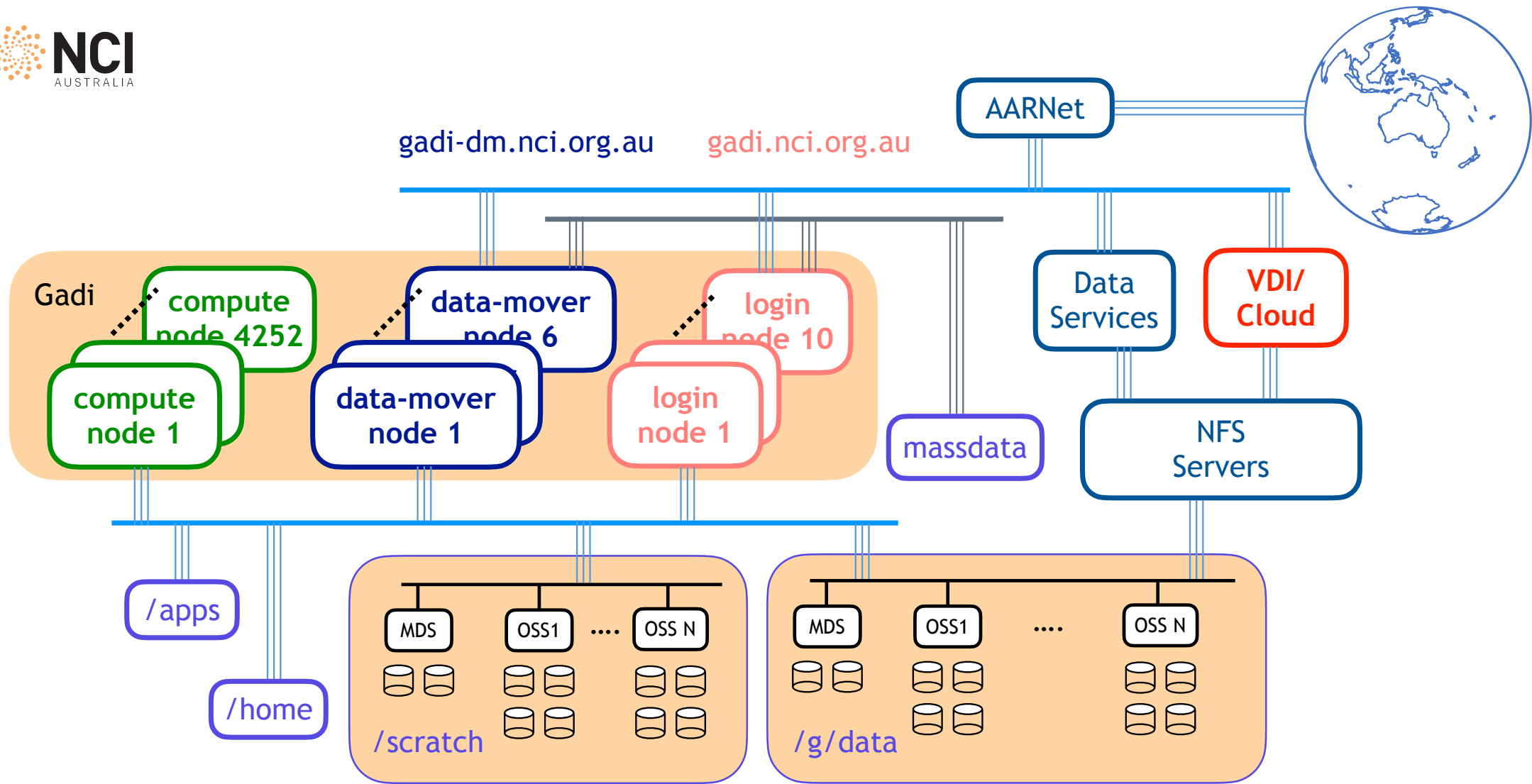


Gadi



Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)
27	Gadi - PRIMERGY CX2570 M5, ThinkSystem SD650, Xeon Platinum 8274/8268, NVIDIA Tesla V100 SXM2, Mellanox HDR Infiniband, Fujitsu / Lenovo National Computational Infrastructure (NCI Australia) Australia	204,032	9,264.3	15,142.2

<https://www.top500.org/lists/top500/list/2020/11/>



Gadi

- Access to more CPU, GPU, memory, storage and faster interconnect between them
 - CPU cores: (Cascade Lake, 155K), (Broadwell, 23K), (Skylake, 6K)
 - GPUs: 160*4 NVIDIA V100
 - High memory: (4*clx, 3TiB), (50*clx, 1.5TiB), (3*bdw, 3TiB), (10*bdw, 1TiB)
 - Parallel file systems: (/scratch, 11PiB)*2, (/g/data, ~11PiB)*4, (massdata, 25PiB)*2 extensible to 100 PiB each.
- Application software catalogue
 - MPI compiled for utilising the faster interconnections
 - Python3, R, Julia compiled with libraries such as intel-mkl, FFTW, and possibility to build your own packages
 - Matlab for almost all major research universities, like ANU, UNSW, RMIT, Monash, USyd, Macquarie...
 - Deep Learning Frameworks: tensorflow, pytorch

Gadi

- Shared resources
 - Read and write operations to and from the shared file systems
 - For jobs use less than a full compute node
- Gadi runs under CentOS 8.3.2011 as of 28 April 2021
- Most applications for scientific computing support CentOS/RHEL
- No root privilege like you have on your local Ubuntu/MacOS/Windows
 - Installation goes to your project/home directories, not the default system directories like /bin
 - Ask for help when changing file/directory ownership and permission
- Not Ideal for GUI, but possible with X forwarding enabled
- 48 hours default limit for normal queue jobs using less than 720 CPU cores*

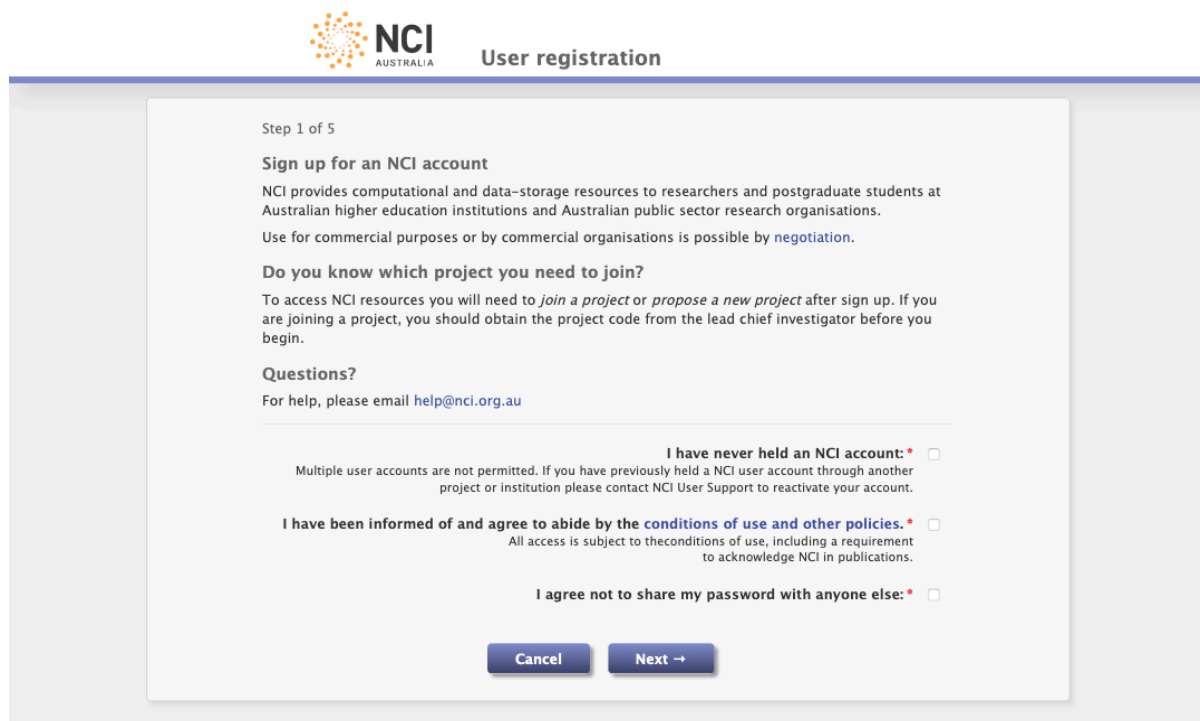
* walltime limit varies and exception can be granted if necessary, see details here <https://opus.nci.org.au/display/Help/Queue+Limits>



Get Access

User, Project and Stakeholder

User Registration at my.nci.org.au



Step 1 of 5

Sign up for an NCI account

NCI provides computational and data-storage resources to researchers and postgraduate students at Australian higher education institutions and Australian public sector research organisations. Use for commercial purposes or by commercial organisations is possible by [negotiation](#).

Do you know which project you need to join?

To access NCI resources you will need to *join a project* or *propose a new project* after sign up. If you are joining a project, you should obtain the project code from the lead chief investigator before you begin.

Questions?
For help, please email help@nci.org.au

I have never held an NCI account: *
Multiple user accounts are not permitted. If you have previously held a NCI user account through another project or institution please contact NCI User Support to reactivate your account.

I have been informed of and agree to abide by the conditions of use and other policies. *
All access is subject to the conditions of use, including a requirement to acknowledge NCI in publications.

I agree not to share my password with anyone else: *

Follow the registration dialogue:

- Confirm no previous account
- Provide your details:
 - Institution email address
 - Mobile number
 - Institution
- Project code

* see more details here

<https://opus.nci.org.au/display/Help/1.0.0+User+Account+Registration>

Propose Project after User Registration



Yue Sun | Log out

Home → Propose project → Step 5

Overview
About me
Change password
Projects and groups
Propose a project

Step 5 of 10

Choose an allocation scheme

The allocation schemes listed below are available to users at your research institution. Select the scheme to which you wish to apply.

- NCI Startup**
NCI Startup projects provide modest Gadi compute allocations of up to 2 KSU/quarter for a calendar year. They are intended to help researchers evaluate the suitability of NCI for their research and to assist in developing capability, expertise and a facility track record in support of applications for more substantial resources through merit and partner allocation schemes.
Administrator: Roger Edberg (NCI staff)
Available resources:
 - Gadi: compute

...

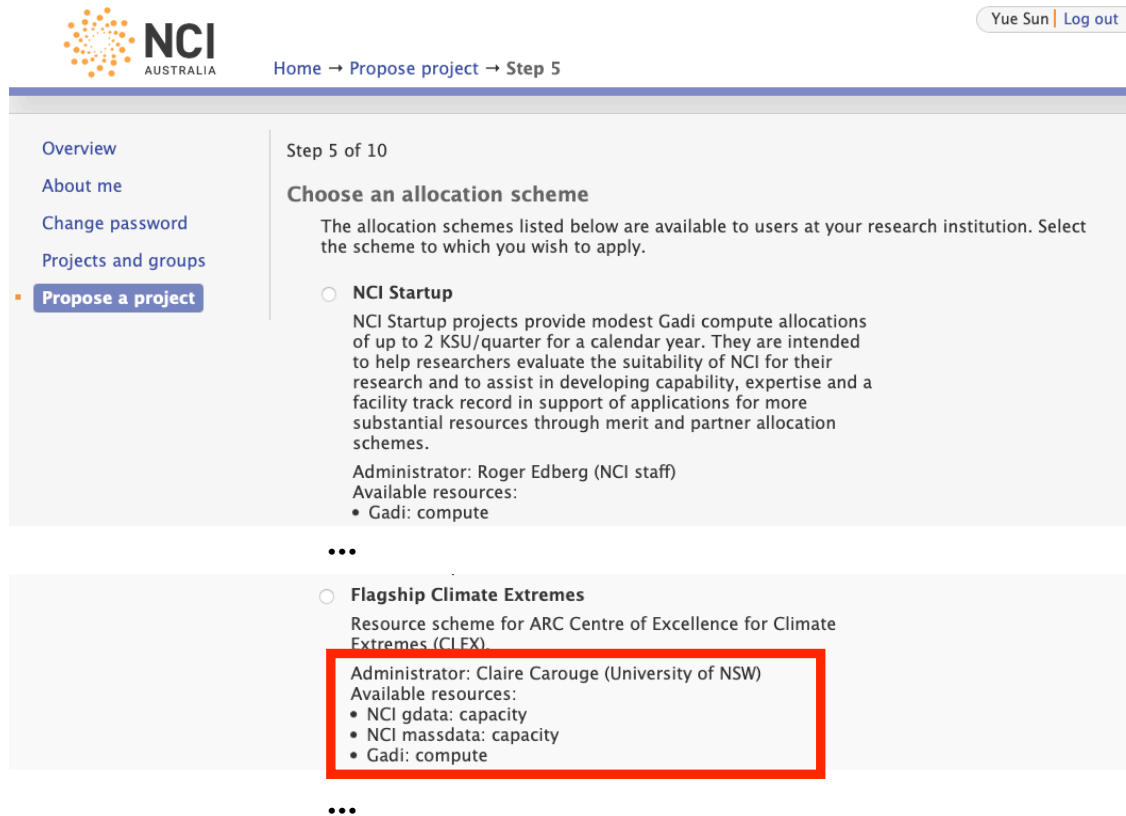
- Flagship Climate Extremes**
Resource scheme for ARC Centre of Excellence for Climate Extremes (CLEX).
Administrator: Claire Carouge (University of NSW)
Available resources:
 - NCI gdata: capacity
 - NCI massdata: capacity
 - Gadi: compute

...

Steps:

- Acknowledge Terms and Conditions of Use
- Write project proposal
 - Project description
 - Research field classification
 - Resources request
- Choose which scheme to propose to
- Invite project members on board

Propose Project after User Registration



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Available resources:
 - Gadi: compute
- ...
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Resource scheme for ARC Centre of Excellence for Climate Extremes (CLFX).
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Available resources:
 - NCI gdata: capacity
 - NCI massdata: capacity
 - Gadi: compute
- ...

Steps:

- Acknowledge Term and Conditions of Use
- Write the proposal
 - Project description
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 - Resources request
- Choose which scheme to propose to
- Invite project members on board

Current Stakeholders

- Universities: ANU, UNSW, Sydney, Melbourne, RMIT, Monash, Deakin, UQ, Adelaide, Macquarie, Wollongong, UTS, UTAS, Victoria University
- Australian Government research agencies, Bureau of Meteorology, CSIRO, and Geoscience Australia
- ARC Centres of Excellence, CLEX, FLEET, Exciton Science
- Consortia: QCIF, Intersect
- Merit schemes: NCMAS, ALCG



Showcase
Login

Login to Gadi

- a. Open a terminal and login to one of the ten login nodes by doing

```
ssh <jjj777>@gadi.nci.org.au
```

Your username goes here

- b. X forwarding enabled login and test with xeyes

```
Sue@local:~ $ ssh -Y jjj777@gadi.nci.org.au
jjj777@gadi.nci.org.au's password:
[jjj777@gadi-login-05 ~]$ xeyes
[jjj777@gadi-login-05 ~]$ exit
Sue@local:~ $
```



Showcase

Basic Application Workflow on Gadi

A horizontal banner image showing a colorful, abstract representation of microscopic tissue sections, likely stained with various dyes to highlight different cellular structures and components.

Showcase

Submit and Monitor Jobs

Submit Jobs and Monitor Status

```
qsub gutentag.sh  
qstat -u $USER -sw  
qstat -fx <jobid>  
cat <jobname>.o<jobid>
```

```
$ qsub gutentag.sh
21715720.gadi-pbs
$ qstat -u $USER -sw
```

```
gadi-pbs:
```

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	Elap S Time
21715720.gadi-pbs	xyz123	copyq-exec	gutentag.sh	591715	1	1	2048m	02:00	R 00:00

Job run at Thu Apr 29 at 13:02 on (gadi-dm-01:ncpus=1:mem=2097152kb:jobfs=102400kb)

```
$
$
$
$
$
$
$
```

```
$ qstat -fx 21715720
```

```
Job Id: 21715720.gadi-pbs
Job_Name = gutentag.sh
Job_Owner = xyz123@gadi-login-09.gadi.nci.org.au
resources_used.cput = 0
resources_used.jobfs = 0b
resources_used.mem = 185664kb
resources_used.ncpus = 1
resources_used.vmem = 185664kb
resources_used.walltime = 00:00:01
job_state = E
queue = copyq-exec
server = gadi-pbs-01.gadi.nci.org.au
Checkpoint = u
ctime = Thu Apr 29 13:01:08 2021
Error_Path = gadi.nci.org.au:/home/123/xyz123/training/IntroGadi/gutentag.sh.e21715720
exec_host = gadi-dm-01/21
exec_vnode = (gadi-dm-01:ncpus=1:mem=2097152kb:jobfs=102400kb)
group_list = c25
Hold_Types = n
Join_Path = n
Keep_Files = n
Mail_Points = a
mtime = Thu Apr 29 13:02:24 2021
Output_Path = gadi.nci.org.au:/home/123/xyz123/training/IntroGadi/gutentag.sh.o21715720
Priority = 0
qtime = Thu Apr 29 13:01:08 2021
Rerunnable = False
Resource_List.jobfs = 104857600b
Resource_List.jobprio = 11
Resource_List.mem = 2147483648b
Resource_List.mpiexecs = 1
Resource_List.ncpus = 1
Resource_List.nodect = 1
Resource_List.place = free
Resource_List.select = 1:ncpus=1:mpiprocs=1:mem=2147483648:job_tags=copyq:jobfs=104857600
Resource_List.storage = scratch/ab01+gdata/ab01
Resource_List.uuid = d03c83ae-be30-406a-baf6-5541ab91748a
Resource_List.walltime = 02:00:00
Resource_List.wd = 1
stime = Thu Apr 29 13:02:03 2021
session_id = 591715
jobdir = /home/123/xyz123
substate = 53
Variable_List = PBS_O_HOME=/home/900/yxs900,PBS_O_LANG=en_AU.UTF-8,
PBS_O_LOGNAME=yxs900,
PBS_O_PATH=/opt/pbs/default/bin:/opt/nci/bin:/opt/bin:/opt/Modules/v4.3.0/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/pbs/default/bin,
PBS_O_MAIL=/var/spool/mail/xyz123,PBS_O_SHELL=/bin/bash,
PBS_O_TZ=/etc/localtime,
PBS_O_WORKDIR=/home/123/xyz123/training/IntroGadi,PBS_O_SYSTEM=Linux,
PROJECT=c25,PBS_NCI_HT=0,
PBS_NCI_STORAGE=scratch/ab01+gdata/ab01,PBS_NCI_IMAGE=,
PBS_NCPUS=1,PBS_NGPUS=0,PBS_NNODES=1,PBS_NCI_NCPUS_PER_NODE=48,
PBS_NCI_NUMA_PER_NODE=4,PBS_NCI_NCPUS_PER_NUMA=12,PBS_VMEM=2147483648,
PBS_NCI_WD=1,PBS_NCI_JOBFS=104857600b,PBS_NCI_LAUNCH_COMPATIBILITY=0,
PBS_NCI_FS_GDATA1=0,PBS_NCI_FS_GDATA1A=0,PBS_NCI_FS_GDATA1B=0,
PBS_NCI_FS_GDATA2=0,PBS_NCI_FS_GDATA3=0,PBS_NCI_FS_GDATA4=0,
PBS_O_QUEUE=copyq,PBS_O_HOST=gadi-login-09.gadi.nci.org.au,
PBS_JOBFS=/jobfs/21715720.gadi-pbs
comment = Job run at Thu Apr 29 at 13:02 on (gadi-dm-01:ncpus=1:mem=2097152kb:jobfs=102400kb)
etime = Thu Apr 29 13:01:08 2021
run_count = 1
Stageout_status = 1
Exit_status = 0
Submit_arguments = gutentag.sh
project = ab01
Submit_Host = gadi-login-09.gadi.nci.org.au
```

```
$
$
$
$
$
```

```
$ cat gutentag.sh
#!/bin/bash
```

```
#PBS -P ab01
#PBS -q copyq
#PBS -l ncpus=1
#PBS -l mem=2GB
#PBS -l walltime=02:00:00
#PBS -l storage=scratch/ab01+gdata/ab01
#PBS -l wd
```

```
hostname
```

```
export DSTDIR=/g/data/ab01/xyz123/job_archive
export SOURCEDIR=/scratch/ab01/xyz123/benchmarks/python/tensorflow
```

```
cp -vr $SOURCEDIR $DSTDIR > ${PBS_JOBID}.log
```

```
$
$
$
$
$
```

```
$ cat gutentag.sh.o21715720
gadi-dm-01.gadi.nci.org.au
```

```
=====
Resource Usage on 2021-04-29 13:02:41:
```

Job Id:	21715720.gadi-pbs	
Project:	ab01	
Exit Status:	0	
Service Units:	0.00	
NCPUs Requested:	1	NCPUs Used: 1
		CPU Time Used: 00:00:00
Memory Requested:	2.0GB	Memory Used: 181.31MB
Walltime requested:	02:00:00	Walltime Used: 00:00:01
JobFS requested:	100.0MB	JobFS used: 0B

```
=====
```

Job Submission Script

```
#!/bin/bash
```

```
#PBS -P ab01
```

Project Ownership

```
#PBS -q copyq
```

```
#PBS -l ncpus=1
```

```
#PBS -l mem=2GB
```

```
#PBS -l walltime=02:00:00
```

Resource Requests → Reserved SU

```
#PBS -l storage=scratch/ab01+gdata/ab01
```

```
#PBS -l wd
```

```
hostname
```

```
export DSTDIR=/g/data/ab01/xyz123/job_archive
```

```
export SOURCEDIR=/scratch/ab01/xyz123/benchmarks/python/tensorflow
```

```
cp -vr $SOURCEDIR $DSTDIR > ${PBS_JOBID}.log
```


Job Submission Script

```
#!/bin/bash
#PBS -P ab01
#PBS -q copyq
#PBS -l ncpus=1
#PBS -l mem=2GB
#PBS -l walltime=02:00:00
#PBS -l storage=scratch/ab01+gdata/ab01
#PBS -l wd
```

```
hostname
export DSTDIR=/g/data/ab01/xyz123/job_archive
export SOURCEDIR=/scratch/ab01/xyz123/benchmarks/python/tensorflow
cp -vr $SOURCEDIR $DSTDIR > ${PBS_JOBID}.log
```

Actual Tasks: hostname, cp
Run your own applications

Submit an Interactive Job

```
qsub -I -lstorage=gdata/c25+scratch/x11,wd job.sh
```

- Add PBS directives so that the job
 - sends you email at start: `-M <abc123>@<gmail.com> -m abe`
 - waits until matlab licenses is available: `-lsoftware=matlab_<unsw>`
 - redirects STDOUT and STDERR into the specific log(s):
 - `-e err.log -o /scratch/c25/abc123/Logs/`
 - `-j eo`
 - waits until 1:55pm to start: `-a 202105111355`

Extended Reading <https://opus.nci.org.au/display/Help/PBS+Directives+Explained>



Showcase

Monitor Project Usage

\$ nci_account -P ab01

Usage Report: Project=ab01 Period=2021.q2

```
=====
Grant:    471.00 KSU
Used:    406.30 KSU
Reserved:  0.00 SU
Avail:    64.70 KSU
```

Storage Usage Report: Project=ab01

```
=====
Filesystem      Used      iUsed      Allocation  iAllocation
gdata1a         513.57 GB  6.00       2.00 TB     312.00 K
=====
```

\$
\$
\$
\$
\$
\$

\$ nci_account -P ab01 -p 2021.q1

Usage Report: Project=ab01 Period=2021.q1

```
=====
Grant:    548.00 KSU
Used:    524.56 KSU
Reserved:  0.00 SU
Avail:    23.44 KSU
```

Storage Usage Report: Project=ab01

```
=====
Filesystem      Used      iUsed      Allocation  iAllocation
gdata1b         513.57 GB  6.00       2.00 TB     312.00 K
=====
```

\$
\$
\$
\$
\$
\$

\$ nci_account -P ab01 -p 2021.q1 -v

Usage Report: Project=ab01 Period=2021.q1

```
=====
Grant:    548.00 KSU
Used:    524.56 KSU
Reserved:  0.00 SU
Avail:    23.44 KSU
```

```
-----
Stakeholder      Grant      Used      Avail
-----
MAS               250.00 KSU  249.65 KSU  354.93 SU
UNSW              298.00 KSU  274.92 KSU  23.08 KSU
-----
```

```
-----
User              Used      Reserved
-----
abc321            372.50 KSU  0.00 SU
xyz123            152.06 KSU  0.00 SU
-----
```

Storage Usage Report: Project=a57

```
=====
Filesystem      Used      iUsed      Allocation  iAllocation
gdata1b         513.57 GB  6.00       2.00 TB     312.00 K
```

```
-----
Stakeholder      Allocation  iAllocation
-----
UNSW              2.00 TB     312.00 K
-----
```

Monitoring Grant and Usage

- Project can receive compute/storage grant from multiple schemes
- One SU
 - supports a single CPU core job submitted to normal queue with up to 4GiB memory request to run for 30 minutes
 - has the nominal value of 4 cents for grant application purpose
- Storage
 - 72 GB /scratch/\$PROJECT by default, more available to meet job demand, auto-purge policy applied
 - /g/data/\$PROJECT needs approval from scheme managers

Extended Reading <https://opus.nci.org.au/display/Help/2.2+Job+Cost+Examples>

```
$ nci-files-report -f scratch --group xy12
```

FILESYSTEM	SCAN DATE	PROJECT	GROUP	USER	SPACE USED	TOTAL SIZE	COUNT
scratch	2020-12-27	am1	xy12	xyz123	2.0G	2.0G	3968
scratch	2020-12-27	ab01	xy12	xyz123	48.0K	11.8K	21
scratch	2020-12-27	ab01	xy12	abc321	32.0K	4.8K	12
scratch	2020-12-27	xy12	xy12	xyz123	396.0K	211.8K	97
scratch	2020-12-27	xy12	xy12	abc321	29.7G	29.7G	7258

```
$ nci-files-report -f scratch --project xy12
```

FILESYSTEM	SCAN DATE	PROJECT	GROUP	USER	SPACE USED	TOTAL SIZE	COUNT
scratch	2020-12-27	xy12	c25	xyz123	2.7G	2.7G	1652
scratch	2020-12-27	xy12	xy12	xyz123	396.0K	211.8K	97
scratch	2020-12-27	xy12	xy12	abc321	29.7G	29.7G	7258

```
$ nci-files-report -f scratch --user xyz123
```

FILESYSTEM	SCAN DATE	PROJECT	GROUP	USER	SPACE USED	TOTAL SIZE	COUNT
scratch	2020-12-27	am1	xy12	xyz123	2.0G	2.0G	3968
scratch	2020-12-27	ab01	xy12	xyz123	48.0K	11.8K	21
scratch	2020-12-27	xy12	c25	xyz123	2.7G	2.7G	1652
scratch	2020-12-27	xy12	xy12	xyz123	396.0K	211.8K	97

A horizontal banner image showing a colorful, abstract microscopic view of tissue, likely stained with various dyes to highlight different cellular structures and components.

Showcase

Use Applications installed on /apps

Module Environment

- Multiple versions and conflicting packages
- module commands
 - module avail python3
 - module list
 - module show python3/3.9.2
 - module load python3/3.9.2
 - module unload python3


```
$ module avail python3
-----/apps/Modules/modulefiles -----
python3-as-python  python3/3.7.4  python3/3.8.5  python3/3.9.2
```

```
$ module list
Currently Loaded Modulefiles:
 1) pbs
```

```
$ module show python3/3.9.2
-----
/apps/Modules/modulefiles/python3/3.9.2:

prepend-path      PATH /apps/python3/3.9.2/bin
prepend-path      C_INCLUDE_PATH /apps/python3/3.9.2/include/python3.9
prepend-path      CPLUS_INCLUDE_PATH /apps/python3/3.9.2/include/python3.9
prepend-path      CPATH /apps/python3/3.9.2/include/python3.9
prepend-path      FPATH /apps/python3/3.9.2/include/python3.9
prepend-path      LIBRARY_PATH /apps/python3/3.9.2/lib
prepend-path      LD_LIBRARY_PATH /apps/python3/3.9.2/lib
prepend-path      LD_RUN_PATH /apps/python3/3.9.2/lib
prepend-path      MANPATH /apps/python3/3.9.2/share/man
prepend-path      PKG_CONFIG_PATH /apps/python3/3.9.2/lib/pkgconfig
module            load intel-mkl/2020.3.304
conflict          python3
setenv            PYTHON3_BASE /apps/python3/3.9.2
setenv            PYTHON3_ROOT /apps/python3/3.9.2
setenv            PYTHON3_VERSION 3.9.2
module-whatis    {python3, version 3.9.2}
-----
```

```
$ module load python3/3.9.2
Loading python3/3.9.2
  Loading requirement: intel-mkl/2020.3.304
```

```
$ module list
Currently Loaded Modulefiles:
 1) pbs  2) intel-mkl/2020.3.304  3) python3/3.9.2
```

```
$ python3
Python 3.9.2 (default, Mar 29 2021, 10:41:26)
[GCC 8.3.1 20191121 (Red Hat 8.3.1-5)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> np.__version__
'1.20.0'
>>> exit()
```

```
$ module load python3/3.8.5
MODULE ERROR DETECTED: GLOBALERR python3/3.8.5 cannot be loaded due to a
conflict.
(Detailed error information and backtrace has been suppressed, set
$MODULES_ERROR_BACKTRACE to unsuppress.)
```

```
Loading python3/3.8.5
ERROR: python3/3.8.5 cannot be loaded due to a conflict.
HINT: Might try "module unload python3" first.
```

Software Catalogue

- Modules on Gadi are named as `<software>/<version>`
 - always load a specific version of the software application under interest
 - ``module load <software>`` loads the default version which changes over time
- ``module load`` does the following
 - modifies search/exec path
 - loads prerequisite modules [intel-mkl/2020.3.304 for python3/3.9.2]
 - handles software/module conflicts
 - configures environment to define how the application runs

Software Groups

- Restricted Modules are available to specific groups of users
- Software groups control access to license modules
 - Try: `module avail matlab`
- License Modules tell the application where to checkout license

```
$ module avail matlab
-----/apps/Modules/restricted-modulefiles/matlab_anu -----
matlab_licence/anu

-----/apps/Modules/restricted-modulefiles/matlab_usyd -----
matlab_licence/usyd

-----/apps/Modules/restricted-modulefiles/matlab_vu -----
matlab_licence/vu

-----/apps/Modules/restricted-modulefiles/matlab_utas -----
matlab_licence/utas

-----/apps/Modules/modulefiles -----
matlab/R2019b  matlab/R2020b
```

```
$ getfacl /apps/Modules/restricted-modulefiles/matlab_anu
getfacl: Removing leading '/' from absolute path names
# file: apps/Modules/restricted-modulefiles/matlab_anu
# owner: apps
# group: z30
user::rwx
group::rwx
group:matlab_anu:r-x
mask::rwx
other:---
```

```
$ module show matlab_licence/anu
-----
/apps/Modules/restricted-modulefiles/matlab_anu/matlab_licence/anu:

setenv          MLM_LICENSE_FILE 12345678@xxxxxxxxx.anu.edu.au
conflict        matlab_licence
module-whatis   {matlab_licence, version anu}
-----
```

```
$ module load matlab/R2020b
$ module load matlab_licence/anu
$ matlab -nodesktop -nodisplay
```

```
< M A T L A B (R) >
Copyright 1984-2020 The MathWorks, Inc.
R2020b Update 5 (9.9.0.1592791) 64-bit (glnxa64)
February 4, 2021
```

```
To get started, type doc.
For product information, visit www.mathworks.com.
```

```
>> eig(magic(3))
```

```
ans =

    15.0000
     4.8990
    -4.8990
```

```
>> exit()
```

```
$ ls
test.m
$ matlab -nodesktop -nodisplay -r "var1='$PBS_JOBFS',var2=$PBS_NCPUS, test, exit"
```

Showcase

Build Your Own Python/R/Julia Packages on Gadi

Example I: python3 pandas

```
module purge
module load python3/3.9.2
InstallDir=/scratch/$PROJECT/$USER/.local/python
mkdir -p $InstallDir
pip3 install -v --no-binary :all: -prefix=$InstallDir pandas

export PYTHONPATH=$InstallDir/lib/python3.9/site-packages:$PYTHONPATH
python3
>>> import pandas as pd
```

```

$ module list
Currently Loaded Modulefiles:
 1) pbs
$ module load python3/3.9.2
Loading python3/3.9.2
  Loading requirement: intel-mkl/2020.3.304
$ module list
Currently Loaded Modulefiles:
 1) pbs  2) intel-mkl/2020.3.304  3) python3/3.9.2
$
$
$
$
$
$
$ python3
Python 3.9.2 (default, Mar 29 2021, 10:41:26)
[GCC 8.3.1 20191121 (Red Hat 8.3.1-5)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
>>>
>>>
>>>
>>>
>>> import numpy as np
>>> np.__file__
'/apps/python3/3.9.2/lib/python3.9/site-packages/numpy-1.20.0-py3.9-linux-
x86_64.egg/numpy/__init__.py'
>>>
>>>
>>>
>>>
>>> import multiprocessing
>>> multiprocessing.__file__
'/apps/python3/3.9.2/lib/python3.9/multiprocessing/__init__.py'
>>>
>>>
>>>
>>>
>>> import pandas as pd
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'pandas'
>>> exit()
$
$
$
$
$
$
$ InstallDir=/scratch/$PROJECT/$USER/.local/python
$ mkdir -p $InstallDir
$ pip3 install -v --no-binary :all: --prefix=$InstallDir pandas >
pandas_build.log
.
.
.
$ grep -i succ pandas_build.log
Successfully built pandas
Successfully installed pandas-1.2.4 pytz-2021.1
$ ls $InstallDir/lib/python3.9/site-packages/
pandas pandas-1.2.4.dist-info pytz pytz-2021.1-py3.9.egg-info
$
$
$
$
$
$
$ export PYTHONPATH=$InstallDir/lib/python3.9/site-packages:$PYTHONPATH
$ python3
Python 3.9.2 (default, Mar 29 2021, 10:41:26)
[GCC 8.3.1 20191121 (Red Hat 8.3.1-5)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import pandas as pd
>>> pd.__file__
'/scratch/ab01/xyz123/.local/python/lib/python3.9/site-packages/pandas/
__init__.py'
>>>

```

Example II: python3 neural-structured-learning

```
module purge
module load tensorflow/2.4.1
pip3 install -v --no-binary :all: --prefix=$InstallDir neural-structured-learning==1.2.0

python3
>>> import neural_structured_learning as nsl
```



```
$ module purge
$ module load tensorflow/2.4.1
Loading tensorflow/2.4.1
  Loading requirement: intel-mkl/2020.3.304 python3/3.9.2 cuda/11.0.3 cudnn/8.1.1-cuda11 nccl/2.8.4-
cuda11.0 openmpi/4.0.3
$ module list
Currently Loaded Modulefiles:
 1) intel-mkl/2020.3.304   3) cuda/11.0.3           5) nccl/2.8.4-cuda11.0   7) tensorflow/2.4.1
 2) python3/3.9.2        4) cudnn/8.1.1-cuda11   6) openmpi/4.0.3
$
$
$
$
$
$ echo $InstallDir
/scratch/ab01/xyz123/.local/python
$ pip3 install -v --no-binary :all: --prefix=$InstallDir neural-structured-learning==1.2.0
.
.
.
Successfully installed neural-structured-learning-1.2.0
WARNING: You are using pip version 21.0.1; however, version 21.1.1 is available.
You should consider upgrading via the '/apps/python3/3.9.2/bin/python3.9 -m pip install --upgrade
pip' command.
Removed build tracker: '/scratch/ab01/xyz123/tmp/pip-req-tracker-4a2cicit'
$
$
$
$
$ echo $PYTHONPATH
/apps/tensorflow/2.4.1/lib/python3.9/site-packages:/scratch/ab01/xyz123/.local/python/lib/python3.9/
site-packages:
$ python3
Python 3.9.2 (default, Mar 29 2021, 10:41:26)
[GCC 8.3.1 20191121 (Red Hat 8.3.1-5)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import neural_structured_learning as nsl
2021-05-06 14:08:33.613622: I tensorflow/stream_executor/platform/default/dso_loader.cc:49]
Successfully opened dynamic library libcudart.so.11.0
>>> nsl.__file__
'/scratch/ab01/xyz123/.local/python/lib/python3.9/site-packages/neural_structured_learning/
__init__.py'
>>> nsl.__version__
'1.2.0'
>>>
```

Example III: R randomForest

```
module purge  
module load intel-compiler/2019.5.281  
module load R/4.0.0  
R
```

```
>install.packages("randomForest",repos="https://mirror.aarnet.edu.au/pub/CRAN/")
```

```
...
```

```
lib = "/apps/R/4.0.0/lib64/R/library" is not writable
```

```
Would you like to use a personal library instead? (yes/No/cancel) yes
```

```
Would you like to create a personal library '~/R/x86_64-pc-linux-gnu-library/4.0' to install packages into? (yes/No/cancel) yes
```

```
$ module purge
$ module load intel-compiler/2019.5.281
$ module load R/4.0.0
$ R
```

```
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.
```

```
Natural language support but running in an English locale
```

```
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.
```

```
> install.packages("randomForest", repos="https://mirror.aarnet.edu.au/pub/CRAN/")
Warning in install.packages("randomForest", repos = "https://mirror.aarnet.edu.au/pub/
CRAN/") :
```

```
'lib = "/apps/R/4.0.0/lib64/R/library"' is not writable
Would you like to use a personal library instead? (yes/No/cancel) yes
Would you like to create a personal library
'~/R/x86_64-pc-linux-gnu-library/4.0'
to install packages into? (yes/No/cancel) yes
trying URL 'https://mirror.aarnet.edu.au/pub/CRAN/src/contrib/
randomForest_4.6-14.tar.gz'
Content type 'application/x-gzip' length 80074 bytes (78 KB)
=====
downloaded 78 KB
```

```
* installing *source* package 'randomForest' ...
** package 'randomForest' successfully unpacked and MD5 sums checked
** using staged installation
** libs
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c classTree.c -o classTree.o
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c init.c -o init.o
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c regTree.c -o regTree.o
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c regrf.c -o regrf.o
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c rf.c -o rf.o
ifort -fpic -g -c rfsuf.f -o rfsuf.o
icc -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I/usr/local/include -fpic -g -O2
-c rfutils.c -o rfutils.o
icc -shared -L/apps/R/4.0.0/lib64/R/lib -L/usr/local/lib64 -o randomForest.so
classTree.o init.o regTree.o regrf.o rf.o rfsuf.o rfutils.o -lifport -lifcoremt -limf
-lsvml -lm -lipgo -lirc -lpthread -lirc_s -ldl -L/apps/R/4.0.0/lib64/R/lib -lR
installing to /home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0/00LOCK-randomForest/
00new/randomForest/libs
** R
** data
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
** building package indices
** testing if installed package can be loaded from temporary location
** checking absolute paths in shared objects and dynamic libraries
** testing if installed package can be loaded from final location
** testing if installed package keeps a record of temporary installation path
* DONE (randomForest)
```

```
The downloaded source packages are in
' /scratch/ab01/xyz123/tmp/RtmpIqJUxr/downloaded_packages'
> library(randomForest)
randomForest 4.6-14
Type rfNews() to see new features/changes/bug fixes.
> library()
```

```
Packages in library '/home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0':
```

```
randomForest      Breiman and Cutler's Random Forests for
Classification and Regression
```

```
Packages in library '/apps/R/4.0.0/lib64/R/library':
```

```
base              The R Base Package
boot              Bootstrap Functions (Originally by Angelo Canty
for S)
class             Functions for Classification
cluster          "Finding Groups in Data": Cluster Analysis
Extended Rousseeuw et al.
.
.
.
parallel         Support for Parallel computation in R
```

Example IV: R Rtsne

```
module purge
module load intel-compiler/2019.5.281
module load R/4.0.0
vi ~/.R/Makevars
R
```

```
>install.packages("randomForest",repos="https://mirror.aarnet.edu.au/pub/
CRAN/")
```

```

$ module purge
$ module load intel-compiler/2019.5.281
$ module load R/4.0.0
$
$
$
$ cat ~/.R/Makevars
CC=gcc
CXX=g++
$
$
$ R

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)
.
.
.
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.

> install.packages("Rtsne", repos="https://mirror.aarnet.edu.au/pub/CRAN/")
Installing package into '/home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0'
(as 'lib' is unspecified)
also installing the dependency 'Rcpp'

trying URL 'https://mirror.aarnet.edu.au/pub/CRAN/src/contrib/Rcpp_1.0.6.tar.gz'
Content type 'application/x-gzip' length 2952876 bytes (2.8 MB)
=====
downloaded 2.8 MB

trying URL 'https://mirror.aarnet.edu.au/pub/CRAN/src/contrib/Rtsne_0.15.tar.gz'
Content type 'application/x-gzip' length 67595 bytes (66 KB)
=====
downloaded 66 KB

* installing *source* package 'Rcpp' ...
** package 'Rcpp' successfully unpacked and MD5 sums checked
** using staged installation
** libs
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c api.cpp -o api.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c attributes.cpp -o attributes.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c barrier.cpp -o barrier.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c date.cpp -o date.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c module.cpp -o module.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I../inst/include/ -I/usr/local/include -fpic -g
-O2 -c rcpp_init.cpp -o rcpp_init.o
g++ -shared -L/apps/R/4.0.0/lib64/R/lib -L/usr/local/lib64 -o Rcpp.so api.o attributes.o barrier.o
date.o module.o rcpp_init.o -L/apps/R/4.0.0/lib64/R/lib -lR
installing to /home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0/00LOCK-Rcpp/00new/Rcpp/libs
** R
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
** building package indices
** installing vignettes
** testing if installed package can be loaded from temporary location
** checking absolute paths in shared objects and dynamic libraries
** testing if installed package can be loaded from final location
** testing if installed package keeps a record of temporary installation path
* DONE (Rcpp)
* installing *source* package 'Rtsne' ...
** package 'Rtsne' successfully unpacked and MD5 sums checked
** using staged installation
** libs
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I'/home/123/xyz123/R/x86_64-pc-linux-gnu-library/
4.0/Rcpp/include' -I/usr/local/include -fopenmp -fpic -g -O2 -c RcppExports.cpp -o RcppExports.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I'/home/123/xyz123/R/x86_64-pc-linux-gnu-library/
4.0/Rcpp/include' -I/usr/local/include -fopenmp -fpic -g -O2 -c Rtsne.cpp -o Rtsne.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I'/home/123/xyz123/R/x86_64-pc-linux-gnu-library/
4.0/Rcpp/include' -I/usr/local/include -fopenmp -fpic -g -O2 -c normalize_input.cpp -o
normalize_input.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I'/home/123/xyz123/R/x86_64-pc-linux-gnu-library/
4.0/Rcpp/include' -I/usr/local/include -fopenmp -fpic -g -O2 -c sptree.cpp -o sptree.o
g++ -I"/apps/R/4.0.0/lib64/R/include" -DNDEBUG -I'/home/123/xyz123/R/x86_64-pc-linux-gnu-library/
4.0/Rcpp/include' -I/usr/local/include -fopenmp -fpic -g -O2 -c tsne.cpp -o tsne.o
g++ -shared -L/apps/R/4.0.0/lib64/R/lib -L/usr/local/lib64 -o Rtsne.so RcppExports.o Rtsne.o
normalize_input.o sptree.o tsne.o -L/apps/intel-ct/2019.5.281/mkl/lib/intel64 -lmkl_intel_lp64
-lmkl_intel_thread -lmkl_core -liomp5 -lpthread -lifport -lifcoremt -limf -lsvml -lm -lipgo -lirc
-lpthread -lirc_s -ldl -fopenmp -L/apps/R/4.0.0/lib64/R/lib -lR
installing to /home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0/00LOCK-Rtsne/00new/Rtsne/libs
** R
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
** building package indices
** testing if installed package can be loaded from temporary location
** checking absolute paths in shared objects and dynamic libraries
** testing if installed package can be loaded from final location
** testing if installed package keeps a record of temporary installation path
* DONE (Rtsne)

The downloaded source packages are in
'/scratch/ab01/xyz123/tmp/RtmpfWBjN7/downloaded_packages'

> library()

Packages in library '/home/123/xyz123/R/x86_64-pc-linux-gnu-library/4.0':

randomForest      Breiman and Cutler's Random Forests for
                   Classification and Regression
Rcpp               Seamless R and C++ Integration
Rtsne             T-Distributed Stochastic Neighbor Embedding
                   using a Barnes-Hut Implementation

Packages in library '/apps/R/4.0.0/lib64/R/library':

base              The R Base Package
.
.
.
> quit()
Save workspace image? [y/n/c]: n
$
$
$
$ vi ~/.R/Makevars
$ cat !$
cat ~/.R/Makevars
#CC=gcc
#CXX=g++

```

Example V: Julia NLOpt

```
module purge
module load julia/1.5.3
mkdir -p /g/data/$PROJECT/.julia
export JULIA_DEPOT_PATH=/g/data/$PROJECT/.julia
julia

> ]
(@v1.5) pkg> add NLOpt
```

```
$ module purge
$ module load Julia/1.5.3
Loading julia/1.5.3
Loading requirement: fftw3/3.3.8 intel-mkl/2020.2.254
```

```
$ julia
```

```

      _
     _(_)_
    ( )   ( )   | Documentation: https://docs.julialang.org
     _ _ | _ _ _ |
    | | | | | | | / _ _ |
    | | | | | | | ( _ | |
   _/ | \ _ _ | | \ _ _ | |
  | _/ |

julia> ]
```

```
(@v1.5) pkg>
```

```
(@v1.5) pkg> add NLOpt
Installing known registries into `~/julia`
##### 100.0%
Added registry `General` to `~/julia/registries/General`
Resolving package versions...
Installed NLOpt_jll v2.7.0+0
Installed NLOpt v0.6.2
Installed JSONSchema v0.3.3
Installed MbedTLS v1.0.3
Installed Parsers v1.1.0
Installed Preferences v1.2.1
Installed BenchmarkTools v0.7.0
Installed HTTP v0.9.8
Installed IniFile v0.5.0
Installed MbedTLS_jll v2.16.8+1
Installed CodecZlib v0.7.0
Installed ZipFile v0.9.3
Installed NetworkOptions v1.2.0
Installed OrderedCollections v1.4.0
Installed URIs v1.3.0
Installed JSON v0.21.1
Installed Artifacts v1.3.0
Installed Bzip2_jll v1.0.6+5
Installed Zlib_jll v1.2.11+18
Installed TranscodingStreams v0.9.5
Installed MathProgBase v0.7.8
Installed MutableArithmetics v0.2.18
Installed JLLWrappers v1.3.0
Installed CodecBzip2 v0.7.2
Installed MathOptInterface v0.9.21
Installed TOML v1.0.3
```

```
Downloading artifact: NLOpt
Downloading artifact: MbedTLS
Downloading artifact: Bzip2
Downloading artifact: Zlib
Updating `~/julia/environments/v1.5/Project.toml`
 [76087f3c] + NLOpt v0.6.2
Updating `~/julia/environments/v1.5/Manifest.toml`
 [56f22d72] + Artifacts v1.3.0
 [6e4b80f9] + BenchmarkTools v0.7.0
 [6e34b625] + Bzip2_jll v1.0.6+5
 [523fee87] + CodecBzip2 v0.7.2
 [944b1d66] + CodecZlib v0.7.0
 [cd3eb016] + HTTP v0.9.8
 [83e8ac13] + IniFile v0.5.0
 [692b3bcd] + JLLWrappers v1.3.0
 [682c06a0] + JSON v0.21.1
 [7d188eb4] + JSONSchema v0.3.3
 [b8f27783] + MathOptInterface v0.9.21
 [fdb3010] + MathProgBase v0.7.8
 [739be429] + MbedTLS v1.0.3
 [c8ffd9c3] + MbedTLS_jll v2.16.8+1
 [d8a4904e] + MutableArithmetics v0.2.18
 [76087f3c] + NLOpt v0.6.2
 [079eb43e] + NLOpt_jll v2.7.0+0
 [ca575930] + NetworkOptions v1.2.0
 [bac558e1] + OrderedCollections v1.4.0
 [69de0a69] + Parsers v1.1.0
 [21216c6a] + Preferences v1.2.1
 [fa267f1f] + TOML v1.0.3
 [3bb67fe8] + TranscodingStreams v0.9.5
 [5c2747f8] + URIs v1.3.0
 [a5390f91] + ZipFile v0.9.3
 [83775a58] + Zlib_jll v1.2.11+18
 [2a0f44e3] + Base64
 [ade2ca70] + Dates
 [8ba89e20] + Distributed
 [b77e0a4c] + InteractiveUtils
 [76f85450] + LibGit2
 [8f399da3] + Libdl
 [37e2e46d] + LinearAlgebra
 [56ddb016] + Logging
 [d6f4376e] + Markdown
 [a63ad114] + Mmap
 [44cfe95a] + Pkg
 [de0858da] + Printf
 [3fa0cd96] + REPL
 [9a3f8284] + Random
 [ea8e919c] + SHA
 [9e88b42a] + Serialization
 [6462fe0b] + Sockets
 [2f01184e] + SparseArrays
 [10745b16] + Statistics
 [8dfed614] + Test
 [cf7118a7] + UUIDs
 [4ec0a83e] + Unicode
```

```
(@v1.5) pkg> test NLOpt
Testing NLOpt
Status `~/scratch/ab01/xyz123/tmp/jl_7v8iR5/Project.toml`
 [b8f27783] MathOptInterface v0.9.21
 [fdb3010] MathProgBase v0.7.8
 [76087f3c] NLOpt v0.6.2
 [079eb43e] NLOpt_jll v2.7.0+0
 [8dfed614] Test
Status `~/scratch/ab01/xyz123/tmp/jl_7v8iR5/Manifest.toml`
 [56f22d72] Artifacts v1.3.0
 [6e4b80f9] BenchmarkTools v0.7.0
 [6e34b625] Bzip2_jll v1.0.6+5
 [523fee87] CodecBzip2 v0.7.2
 [944b1d66] CodecZlib v0.7.0
 [cd3eb016] HTTP v0.9.8
 [83e8ac13] IniFile v0.5.0
 [692b3bcd] JLLWrappers v1.3.0
 [682c06a0] JSON v0.21.1
 [7d188eb4] JSONSchema v0.3.3
 [b8f27783] MathOptInterface v0.9.21
 [fdb3010] MathProgBase v0.7.8
 [739be429] MbedTLS v1.0.3
 [c8ffd9c3] MbedTLS_jll v2.16.8+1
 [d8a4904e] MutableArithmetics v0.2.18
 [76087f3c] NLOpt v0.6.2
 [079eb43e] NLOpt_jll v2.7.0+0
 [ca575930] NetworkOptions v1.2.0
 [bac558e1] OrderedCollections v1.4.0
 [69de0a69] Parsers v1.1.0
 [21216c6a] Preferences v1.2.1
 [fa267f1f] TOML v1.0.3
 [3bb67fe8] TranscodingStreams v0.9.5
 [5c2747f8] URIs v1.3.0
 [a5390f91] ZipFile v0.9.3
 [83775a58] Zlib_jll v1.2.11+18
 [2a0f44e3] Base64
 [ade2ca70] Dates
 [8ba89e20] Distributed
 [b77e0a4c] InteractiveUtils
 [76f85450] LibGit2
 [8f399da3] Libdl
 [37e2e46d] LinearAlgebra
 [56ddb016] Logging
 [d6f4376e] Markdown
 [a63ad114] Mmap
 [44cfe95a] Pkg
 [de0858da] Printf
 [3fa0cd96] REPL
 [9a3f8284] Random
 [ea8e919c] SHA
 [9e88b42a] Serialization
 [6462fe0b] Sockets
 [2f01184e] SparseArrays
 [10745b16] Statistics
 [8dfed614] Test
 [cf7118a7] UUIDs
 [4ec0a83e] Unicode
f_1([1.234, 5.678])
f_2([0.8787394664016357, 5.551370325142423])
f_3([0.8262160034228196, 5.043903787432386])
f_4([0.4739440370386794, 4.0767726724255375])
f_5([0.35389779634506047, 3.0308503583016])
f_6([0.33387310647853335, 1.9717933962872487])
f_7([0.3333337209575201, 1.0450874902862517])
f_8([0.33333357431034494, 0.4695027039311135])
f_9([0.333333272332185, 0.3057923933552822])
f_10([0.3333337945750244, 0.2963215980646768])
f_11([0.333333342139688, 0.29629628951338166])
got 0.5443310477213124 at [0.333333342139688, 0.29629628951338166] after 11 iterations (returned XTOL_REACHED)
Test Summary:
| Pass Total
Testing NLP with NLOptSolver(:LD_SLSQP, NaN, 1.0e-7, NaN, 1.0e-7, nothing, 1.0e-7, 0, 0, nothing, 0, nothing, 0) | 7 7
Test Summary:
| Pass Total
Testing NLP on the Rosenbrock function with NLOptSolver(:LN_PRAXIS, NaN, 1.0e-7, NaN, 1.0e-7, nothing, 1.0e-7, 0, 0, nothing, 0) | 5 5
Testing NLOpt tests passed
```

A horizontal band of a colorful, abstract microscopic image, possibly a histological section, with various shades of red, orange, yellow, and blue, showing cellular structures.

Showcase

Monitoring Job Efficiency

Resource Utilisation Rate

```
nqstat_anu <jobID1> <jobID2> ...
```

					%CPU	WallTime	Time Lim	RSS	mem	memlim	cpus
12345678	R	abc123	x11	myTest	33	10:53:56	20:00:00	58.7GB	58.7GB	200GB	96
19145286	R	abc123	x11	atmos_ma	96	01:32:41	03:30:00	369GB	369GB	2625GB	768
19149497	R	abc123	x11	coupled.	84	00:34:25	04:30:00	320GB	320GB	1440GB	720
19149708	R	abc123	x11	netcdf_c	71	00:36:30	02:00:00	12.0GB	12.0GB	12.0GB	1
19150248	R	abc123	x11	atmos_ma	86	00:22:27	03:30:00	345GB	345GB	2625GB	768

If under use, look into the job

qcat -e <jobID>

qps -Lopid,nlwp,lwp,stat,sgi_p,pcpu,cputime,comm <jobID>

- `qcat` : print the job's standard streams
 - -e/-o for standard error/out stream
 - -s for submission script
- `qps` : take a snapshot of the current processes in the job
 - launches a `ps` query on each node hosting the job
 - accepts most flags `ps` would take

```
$ nqstat_anu 12345678
```

				%CPU	WallTime	Time Lim	RSS	mem	memlim	cpus	
12345678	R	abc123	x11	myTest	0	10:59:39	48:00:00	228MB	228MB	180GB	96

```
$ qps -Lopid,nlwp,lwp,stat,sgi_p,pcpu,cputime,comm 12345678
```

```
Node 0 (gadi-cpu-clx-2962):
```

PID	NLWP	LWP	STAT	P	%CPU	TIME	COMMAND
232633	1	232633	Ss	*	0.0	00:00:00	bash
232641	1	232641	S	*	0.0	00:00:00	pbs_demux
232682	1	232682	S	*	0.0	00:00:00	12345678.gadi-p
232697	4	232697	Sl	*	0.0	00:00:00	mpirun
232697	4	232702	Sl	*	0.0	00:00:00	mpirun
232697	4	232703	Sl	*	0.0	00:00:00	mpirun
232697	4	232704	Sl	*	0.0	00:00:00	mpirun

```
Node 1 (gadi-cpu-clx-2971):
```

PID	NLWP	LWP	STAT	P	%CPU	TIME	COMMAND
884675	3	884675	Ssl	*	0.0	00:00:00	orted
884675	3	884687	Ssl	*	0.0	00:00:00	orted
884675	3	884688	Ssl	*	0.0	00:00:00	orted

```
$ qcat -e 12345678
```

```
./myTest: error while loading shared libraries: libmkl_intel_lp64.so: cannot open  
shared object file: No such file or directory  
./myTest: error while loading shared libraries: libmkl_intel_lp64.so: cannot open  
shared object file: No such file or directory  
./myTest: error while loading shared libraries: libmkl_intel_lp64.so: cannot open  
shared object file: No such file or directory  
....
```

```
$ qcat -s 12345678
```

```
#!/bin/bash  
#PBS -N myTest  
#PBS -P c25  
#PBS -q normal  
#PBS -l walltime=48:00:00  
#PBS -l mem=180GB  
#PBS -l ncpus=96  
#PBS -l storage=gdata/c25  
#PBS -l wd  
  
module load openmpi/4.0.1  
mpirun -np $PBS_NCPUS ./myTest
```

\$ nqstat_anu 12345679

				%CPU	WallTime	Time Lim	RSS	mem	memlim	cpus	
12345679	R	abc123	x11	myTest	33	10:53:56	48:00:00	58.7GB	58.7GB	180GB	96

\$ myqps 12345679

qps

Node 0 (gadi-cpu-clx-1957):

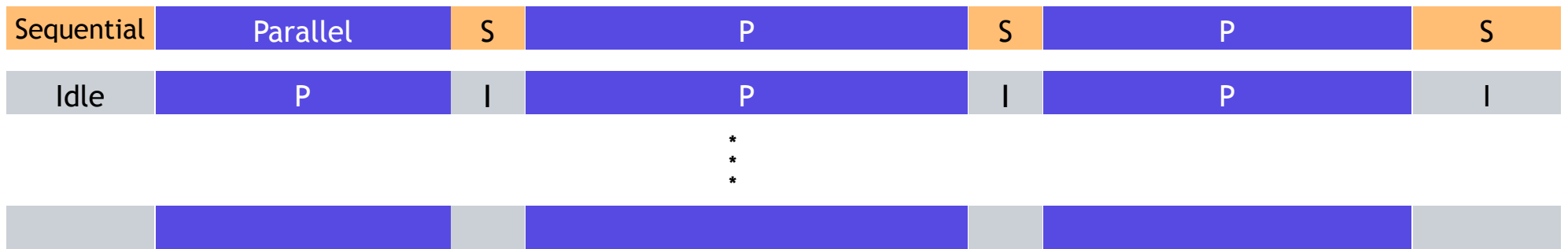
PID	NLWP	LWP	STAT	P	%CPU	TIME	COMMAND
186877	1	186877	Ss	*	0.0	00:00:00	bash
186885	1	186885	S	*	0.0	00:00:00	pbs_demux
186926	1	186926	S	*	0.0	00:00:00	12345679.gadi-p
186961	4	186961	Sl	*	0.0	00:00:00	mpirun
186961	4	186966	Sl	*	0.0	00:00:00	mpirun
186961	4	186967	Sl	*	0.0	00:00:00	mpirun
186961	4	186968	Sl	*	0.0	00:00:00	mpirun
186969	51	186969	Rl	47	90.1	09:56:32	myTest
186969	51	186972	Sl	*	0.0	00:00:00	myTest
186969	51	186975	Sl	*	0.0	00:00:00	myTest
186969	51	186978	Sl	*	0.1	00:00:50	myTest
186969	51	186980	Sl	*	32.6	03:36:20	myTest
186969	51	186981	Sl	*	32.1	03:32:56	myTest
186969	51	186982	Sl	*	32.9	03:38:02	myTest
186969	51	186983	Sl	*	33.1	03:39:17	myTest
186969	51	186984	Sl	*	33.3	03:40:34	myTest
186969	51	186985	Sl	*	32.7	03:37:01	myTest
186969	51	186986	Sl	*	32.9	03:38:07	myTest
186969	51	186987	Sl	*	33.2	03:39:55	myTest
186969	51	186988	Sl	*	32.2	03:33:36	myTest
186969	51	186989	Sl	*	32.1	03:33:06	myTest
186969	51	186990	Sl	*	32.8	03:37:37	myTest
186969	51	186991	Sl	*	33.3	03:40:34	myTest
186969	51	186992	Sl	*	32.8	03:37:33	myTest
186969	51	186993	Sl	*	33.0	03:38:57	myTest
186969	51	186994	Sl	*	32.8	03:37:06	myTest
186969	51	186995	Sl	*	32.7	03:36:59	myTest
186969	51	186996	Sl	*	32.5	03:35:26	myTest
186969	51	186997	Sl	*	32.8	03:37:36	myTest
186969	51	186998	Sl	*	32.7	03:36:36	myTest
186969	51	186999	Sl	*	32.4	03:34:42	myTest
186969	51	187000	Sl	*	31.6	03:29:19	myTest
186969	51	187001	Sl	*	32.6	03:36:03	myTest
186969	51	187002	Sl	*	32.3	03:33:55	myTest
186969	51	187003	Sl	*	33.1	03:39:09	myTest
186969	51	187004	Sl	*	32.7	03:36:36	myTest
186969	51	187005	Sl	*	33.0	03:38:30	myTest
186969	51	187006	Sl	*	33.0	03:38:28	myTest
186969	51	187007	Sl	*	33.2	03:39:45	myTest
186969	51	187008	Sl	*	33.2	03:39:59	myTest
186969	51	187009	Sl	*	32.3	03:34:23	myTest
186969	51	187010	Sl	*	33.8	03:44:10	myTest
186969	51	187011	Sl	*	32.8	03:37:39	myTest
186969	51	187012	Sl	*	33.3	03:40:27	myTest
186969	51	187013	Sl	*	32.5	03:35:44	myTest
186969	51	187014	Sl	*	32.8	03:37:40	myTest
186969	51	187015	Sl	*	32.9	03:38:15	myTest
186969	51	187016	Sl	*	33.3	03:40:45	myTest
186969	51	187017	Sl	*	33.1	03:39:29	myTest
186969	51	187018	Sl	*	32.5	03:35:23	myTest
186969	51	187019	Sl	*	33.0	03:38:32	myTest
186969	51	187020	Sl	*	32.3	03:34:22	myTest
186969	51	187021	Sl	*	32.4	03:34:33	myTest
186969	51	187022	Sl	*	32.7	03:36:36	myTest
186969	51	187023	Sl	*	33.4	03:41:14	myTest
186969	51	187024	Sl	*	33.2	03:40:24	myTest
186969	51	187025	Sl	*	32.1	03:32:52	myTest
186969	51	187026	Sl	*	33.5	03:42:04	myTest

Node 1 (gadi-cpu-clx-1975):

PID	NLWP	LWP	STAT	P	%CPU	TIME	COMMAND
174219	3	174219	SsL	*	0.0	00:00:00	orted
174219	3	174231	SsL	*	0.0	00:00:00	orted
174219	3	174232	SsL	*	0.0	00:00:00	orted
174233	51	174233	Rl	3	88.7	09:47:10	myTest
174233	51	174236	Sl	*	0.0	00:00:00	myTest
174233	51	174239	Sl	*	0.0	00:00:00	myTest
174233	51	174242	Sl	*	0.1	00:00:51	myTest
174233	51	174244	Sl	*	31.5	03:28:34	myTest
174233	51	174245	Sl	*	31.2	03:26:32	myTest
174233	51	174246	Sl	*	31.0	03:25:46	myTest
174233	51	174247	Sl	*	31.5	03:28:41	myTest
174233	51	174248	Sl	*	31.7	03:30:12	myTest
174233	51	174249	Sl	*	31.3	03:27:16	myTest
174233	51	174250	Sl	*	30.9	03:24:32	myTest
174233	51	174251	Sl	*	31.1	03:26:24	myTest
174233	51	174252	Sl	*	31.4	03:27:57	myTest
174233	51	174253	Sl	*	31.1	03:25:51	myTest
174233	51	174254	Sl	*	30.7	03:23:32	myTest
174233	51	174255	Sl	*	31.6	03:29:31	myTest
174233	51	174256	Sl	*	31.6	03:29:31	myTest
174233	51	174257	Sl	*	31.3	03:27:34	myTest
174233	51	174258	Sl	*	31.6	03:29:41	myTest
174233	51	174259	Sl	*	31.5	03:28:43	myTest
174233	51	174260	Sl	*	31.3	03:27:15	myTest
174233	51	174261	Sl	*	31.5	03:28:31	myTest
174233	51	174262	Sl	*	31.4	03:27:50	myTest
174233	51	174263	Sl	*	31.7	03:30:09	myTest
174233	51	174264	Sl	*	31.7	03:29:51	myTest
174233	51	174265	Sl	*	31.4	03:28:21	myTest
174233	51	174266	Sl	*	31.4	03:28:06	myTest
174233	51	174267	Sl	*	31.4	03:28:16	myTest
174233	51	174268	Sl	*	31.3	03:27:45	myTest
174233	51	174269	Sl	*	31.4	03:28:10	myTest
174233	51	174270	Sl	*	31.6	03:29:09	myTest
174233	51	174271	Sl	*	31.6	03:29:38	myTest
174233	51	174272	Sl	*	31.2	03:26:37	myTest
174233	51	174273	Sl	*	31.5	03:28:45	myTest
174233	51	174274	Sl	*	31.6	03:29:41	myTest
174233	51	174275	Sl	*	31.0	03:25:45	myTest
174233	51	174276	Sl	*	31.0	03:25:25	myTest
174233	51	174277	Sl	*	31.0	03:25:37	myTest
174233	51	174278	Sl	*	31.4	03:27:53	myTest
174233	51	174279	Sl	*	31.4	03:28:02	myTest
174233	51	174280	Sl	*	31.0	03:25:15	myTest
174233	51	174281	Sl	*	31.4	03:27:53	myTest
174233	51	174282	Sl	*	31.4	03:28:13	myTest
174233	51	174283	Sl	*	31.4	03:28:18	myTest
174233	51	174284	Sl	*	31.1	03:26:11	myTest
174233	51	174285	Sl	*	31.4	03:27:50	myTest
174233	51	174286	Sl	*	31.3	03:27:44	myTest
174233	51	174287	Sl	*	31.0	03:25:33	myTest
174233	51	174288	Sl	*	31.0	03:25:35	myTest
174233	51	174289	Sl	*	31.3	03:27:22	myTest
174233	51	174290	Sl	*	31.5	03:28:44	myTest

Join-Fork Paradigm

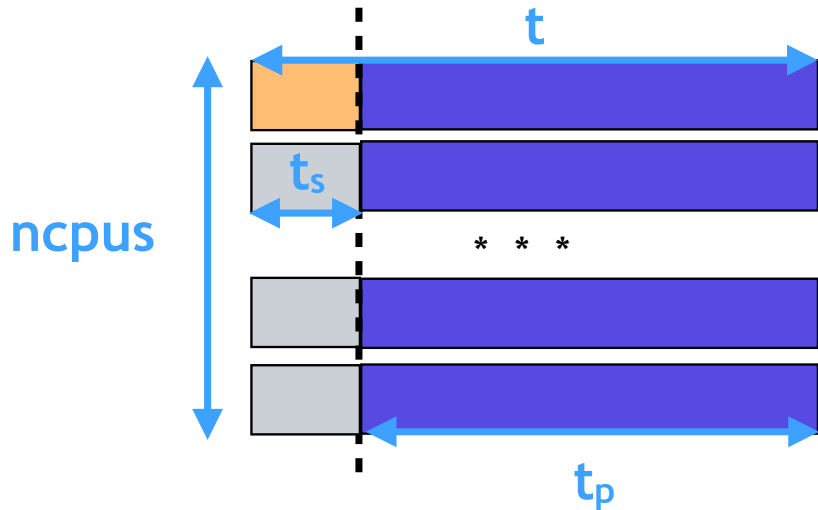
Node 0



Node 1



Theoretical CPU Utilisation Rate in a Ideal Case

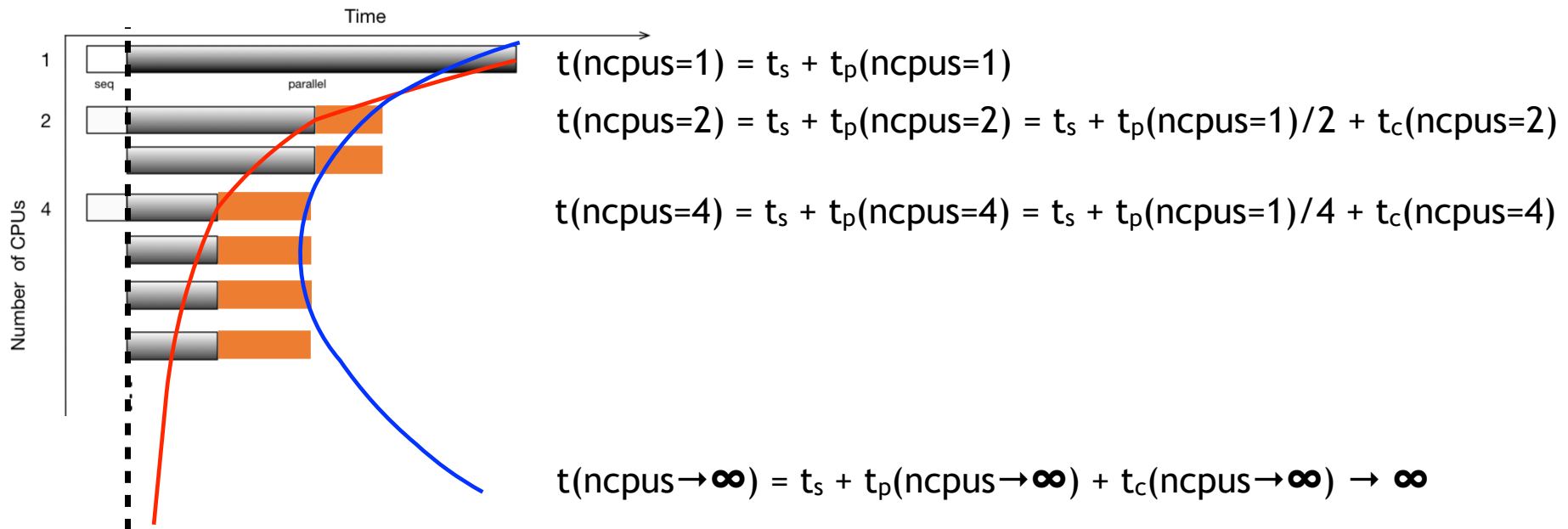


$$\eta(ncpus) = \frac{t_s + ncpus * t_p(ncpus)}{ncpus * t(ncpus)}$$

$\eta(ncpus \rightarrow \infty) \rightarrow 0$
given a constant $ncpus * t_p + t_s$

ncpus	t_p	t	η
1	99	100	1
12	8.25	9.25	0.90
28	3.54	4.54	0.79
48	2.06	3.06	0.68
192	0.52	1.52	0.34

Execution Time Increases Beyond Sweet Spot





Help Desk

Asking Questions

Any More Questions

- Gadi user guide: <https://opus.nci.org.au/display/Help/Gadi+User+Guide>
- User support tickets: help@nci.org.au
- Online support sessions: 1-2pm AEST, first Thursday of each month