AccessDev Transition to Gadi @ https://opus.nci.org.au/display/DAE/UK+Met+Office+Environment+on+NCI NCI



Run Climate and Weather Applications Nonstop For 3 Months

10 November, 2023

Agenda

9:40-9:55	Overview and Highlights	Supported Modes, Timeline, Suite Changes, Ongoing Assistance
10:00-11:00	Work with persistent sessions	Launch a Cylc Job in Localhost Mode from Gadi Login Node
		Morning Tea Break
11:15-12:15	Best Practise Special Notes	Supported Modes, Configuration Changes, Suite Run Directories
		Lunch Break
13:00-14:00	One-Or	n-One: Problem Solving: Rui, Yue, Martin, Dale
14:00-14:30	Known Issue Addressed	SSH configuration, 2-step fcm_make, general porting notes
14:30-15:00	Sharing Suite Progress	Look up Job Progress using Cylc Review in ARE VDI
15:00-15:30	Discussion	How to better support the community • Containerised workflow • Migration to Cylc8 • Other workflows on accessdev •

PAGE TREE

- Overview
- > Al/Machine Learning
- > Data Analysis
- > Bioinformatics and Genomics
- Climate and Weather
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 - Prerequisites
 - > Moving from Accessdev
 - > Workflow meta-scheduler for Cylc suites
 - ✓ Cylc 7
 - Run Cylc7 Suites
 - Develop Cylc7 Suite
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UK Met Office Environment on NCI

Created by Yue Sun, last modified by Ben Evans about 3 hours ago

Many weather and climate models are based on or coupled with the UK Met Office model code, including many of the ACCESS climate and earth systems models, Australian weather model configurations, and the UM suites with coupled model configurations. To support these models, we have created the UK Met Office Environment at NCI.

The environment has been integrated with the system including Gadi, ARE and supporting services. It consists of: the Cylc workflow system; rose suites; the Met Office MOSRS repository and our local replica repository; and the model software and tools.

We note that we are progressively transitioning from the aging **accessdev** environment toward this new Met Office Environment described here.

- Prerequisites
- Moving from Accessdev
 - Accessdev Transition
 - How to migrate your data from accessdev to Gadi
- Workflow meta-scheduler for Cylc suites on ARE/Gadi
 - ARE VDI Sessions for Cylc Jobs
 - Persistent Sessions For Cylc Jobs
 - Sharing Job Progress with Collaborators
- Cylc 7
 - Run Cylc7 Suites



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UKMO Environment Supported

Rose & Cylc workflow software stack (hr22)

- Cylc 7
- Cylc 8
- fcm
- fab
- mosrs-setup

Software repository mirrors (ki32)

- MOSRS
- Nemo
- ...

Spack package manager (ki32)

- Rose/Cylc suite dependencies
- Containerised model packages
- Gitlab CI/CD pipeline*

Computing platforms

- ARE VDI
- ARE JupyterLab
- Persistent Sessions
- Interim special project with the extended PBS time limit

^{*} coming soon

New Home to Cylc Meta-Scheduler

retrieve code load module(s) configure suite run `rose suite-run` manage tasks dependencies
launch tasks
send job submissions
retrieve PBS job status
retrieve job logs
update cylc client

load module(s)
 `cylc gui`
 `cylc review`
monitor workflow

Execute Once

~ 10 minutes

Cylc Meta Scheduler running persistently

~ hours/days/weeks

Every Now and Then

~ 10 minutes









New Home to Cylc Meta-Scheduler



manage tasks dependencies
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update cylc client

Execute Once

~ 10 minutes

Cylc Meta Scheduler running persistently

~ hours/days/weeks

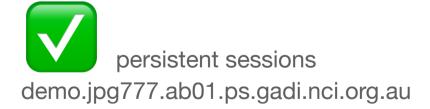
Every Now and Then

~ 10 minutes





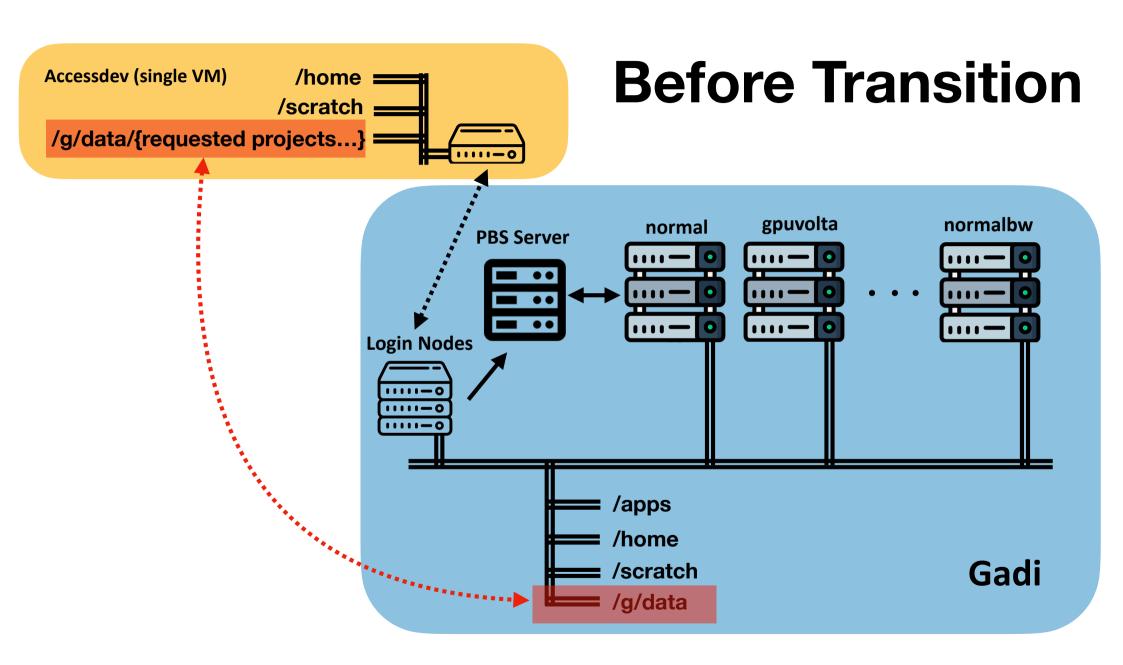


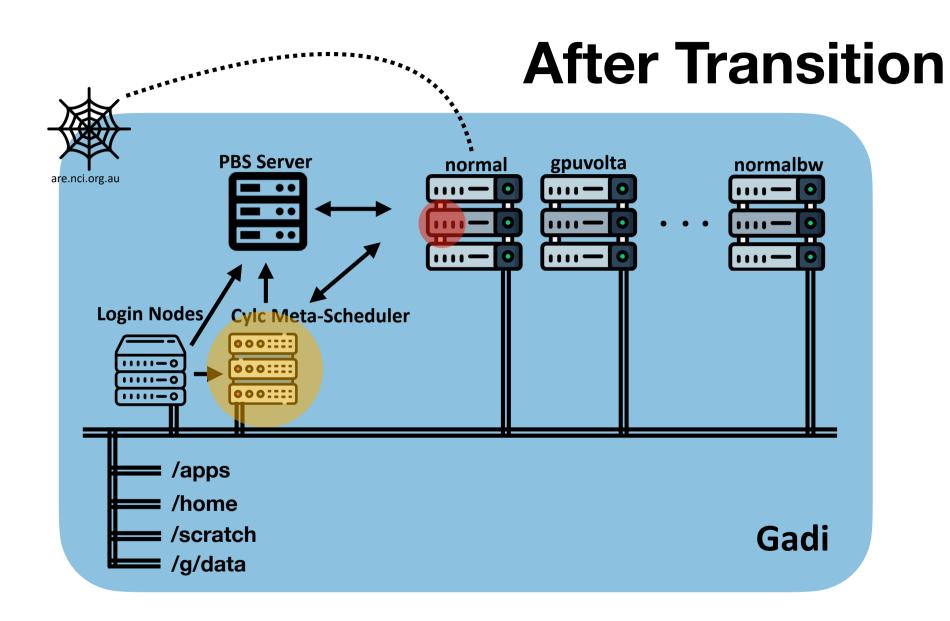




Persistent Sessions @ NCI

- User Specific
- Access to/from Gadi
 - PBS server
 - ARE VDI on compute nodes
 - login nodes
 - /home, /scratch, and /g/data
- Expected Life Span
 - ~ 3 months
 - From maintenance to maintenance





Overview & Highlights

- Supported Modes
- Suite Changes
 - SSH
 - Directories
- Transition Timeline
- Ongoing Assistance
 - Data migration
 - Weekly Open Mic Virtual Lunch
 - NCI Help Desk

Revisit Localhost Mode

- Localhost: Jobs submitted directly from persistent sessions
- Access-Dev Compatible: SSH to login nodes to submit jobs

\$ROSE_ORIG_HOST	Localhost Mode	Access-Dev Compatible Mode
ARE VDI Gadi Login Node	Cylc client on ARE VDI/Login node & server on the persistent session	Special ~/.ssh/config Required Cylc client on ARE VDI/Login node & server on the persistent session
Persistent Session	Both Cylc client & server on the persistent session	Both Cylc client & server on the persistent session

Suite Changes

- Suite Run Directories
 - default to /scratch/\$PROJECT/cylc-run/<suite-id>
 - define user level configuration in
 - `~/.metomi/rose.conf` for Cylc7
 - `~/.cylc/flow/global.cylc` for Cylc8
- Remote Host

 - Change PBS storage options:
 - Add "gdata/hr22+gdata/ki32"

Transition Timeline

- Stages
 - Test runs in PS
 - Production runs in both PS & AD
 - Restricted access to accessdev
 - Decommission of accessdev

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М	Tu	W	Th	F	Sa	Su	М	Tu	W	Th	F	Sa	Su	М	Tu	W	Th	F	Sa	Su
25		27	28	29	30	1	30	31	1	2	3	4	5	27	28	29	30	1	2	3
2	3	4	5	6	7	8	6	7	8	9	10	11	12	4	5	6	1	8	9	10
16	10	11 18	12 19	13 20	14 21	15 22	13 20	14 21	15 22	16 23	17 24	18 25	19 26	11 18	12 19	13 20	14 21	15 22	16 23	17 24
23		25	26	27	28	29	27	28	29	30	1	25	3	25	26	27	28	29	30	31
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M	Tu 2	W 3	4	5	6	7	M 29	Tu 30	W 31	1	2	3	4	M 26	Tu 27	W 28	29 7	1 8	2	3
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M 1 8 15	Tu 2 9 16	W 3 10 17	4 11 18	5 12 19	6 13 20	7 14 21	M 29 5 12	Tu 30 6 13	W 31 7 14	1 8 15	9 16	3 10 17	4 11 18	M 26 4 11	Tu 27 5 12	W 28 6 13 20	29 7 14 21	1 8 15 22	2 9 16 2 23	3 10 17 24

- Key Dates
 - Production runs in persistent sessions supported since 2 Nov
 - Limited access since 1 Feb 2024: only for data access
 - Decommission @ 1 Mar 2024

Ongoing assistance

- Data migration to Gadi
- Open mic starts from 30 Oct @ every Monday 1pm
- NCI Help Desk
 - ticket tag with "accessdev transition"
 - email subject contains "accessdev transition" and cc
 - yue.sun@nci.org.au
 - cws help@nci.org.au





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Run Cylc7/8 suites using Persistent Sessions

- Create a Persistent Session
- Load Modules
- Checkout Suites
- Run Suite

Create a Persistent Session

```
$ persistent-sessions list
                                UUID
                                      PROJECT
                                                    ADDRESS
                                                                 CPUTIME
                                                                           MEMORY
cac76067-5ad0-663c-9791-cfd1c53828f6
                                         ab11
                                                   10.9.4.4 00:30:00.091
                                                                           144.9M
18acc940-e61c-7907-c853-9c9b9013b1ab
                                                   10.9.4.3 00:02:26.939
                                                                           118.8M
                                         ab11
 persistent-sessions start workshopdemo
session d26db958-3238-00db-027b-03ef79cd4acb running - connect using
  ssh workshopdemo.abc111.xy99.ps.gadi.nci.org.au
 persistent-sessions list
                                      PROJECT
                                UUID
                                                    ADDRESS
                                                                 CPUTTMF
                                                                           MEMORY
d26db958-3238-00db-027b-03ef79cd4acb
                                                  10.9.4.12 00:00:00.033
                                                                             3.0M
                                         xy99
cac76067-5ad0-663c-9791-cfd1c53828f6
                                         ab11
                                                                           144.9M
                                                   10.9.4.4 00:30:00.091
18acc940-e61c-7907-c853-9c9b9013b1ab
                                         ab11
                                                   10.9.4.3 00:02:26.939
                                                                           118.8M
 persistent-sessions -h
  persistent-sessions list -h
```

Load Modules

Replace cylc7/23.09 with cylc/8.2.1 if working with Cylc8 suites

```
$ export CYLC_SESSION=workshopdemo.abc111.xy99.ps.gadi.nci.org.au
$ module use /g/data/hr22/modulefiles
$ module load cylc7/23.09
Using the cylc session workshopdemo.abc111.xy99.ps.gadi.nci.org.au
Loading cylc7/23.09
    Loading requirement: mosrs-setup/1.0.1
$ module list
Currently Loaded Modulefiles:
    1) pbs    2) mosrs-setup/1.0.1(default)    3) cylc7/23.09
```

What does the module do?

- env | grep CYLC
- Cylc7: rose config | grep -v ^#
- Cylc8: cylc config -v

Checkout Suites

```
$ mosrs-auth
INFO: You need to enter your MOSRS credentials here so that GPG can
cache your password.
Please enter the MOSRS password for testuser:
INFO: Checking your credentials using Subversion. Please wait.
INFO: Successfully accessed Subversion with your credentials.
INFO: Checking your credentials using rosie. Please wait.
INFO: Successfully accessed rosie with your credentials.
$ rosie co u-cs809
[INFO] u-cs809: local copy created at /home/111/abc111/roses/u-cs809
```

How to redirect the suite run directory to /g/data?

- cat ~/.metomi/rose.conf
- cat ~/.cylc/flow/global.cylc

Run Suites

Replace rose suite-run with cylc install & cylc play <u-cz535> if working with Cylc8 suites

```
$ cd ~/roses/u-cs809
$ rose suite-run
$ readlink ~/cylc-run/u-cs809
/scratch/xy11/abc111/cylc-run/u-cs809
$ readlink ~/cylc-run/u-cz535/runN/log
/scratch/xy11/abc111/cylc-run/u-cz535/run4/log
$ readlink ~/cylc-run/u-cz535/runN/share
/scratch/xy11/abc111/cylc-run/u-cz535/run4/share
$ readlink ~/cylc-run/u-cz535/runN/work
/scratch/xy11/abc111/cylc-run/u-cz535/run4/work
```

What happens next?

- ps auwxff | grep \$USERNAME
- ssh \$CYLC_SESSION "ps auwxff" | grep \$USERNAME

Back @ 11:15



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Best Practise Special Notes

- ROSE_ORIG_HOST and meta-scheduler
- Supported Cylc 7 Suite Modes
- Hands-on excises
- Advanced excises
- FAQ

ROSE_ORIG_HOST and meta-scheduler

- ROSE_ORIG_HOST: The name of the host where the 'rose suite-run' or 'cylc install' command was invoked.
 - Gadi login node or ARE VDI
 - ssh -X gadi.nci.org.au
 - Persistent session (from Gadi login node or ARE VDI)
 - ssh -Y <name>.\$USER.\$PROJECT.ps.gadi.org.au
- Metascheduler: The host executing the cylc main process. It always utilises persistent session specified by
 - \$CYLC SESSION or
 - ~/.persistent-sessions/cylc-session.

Supported Cylc 7 Suite Modes

Accessdev	Gadi: Login nodes, ARE VDI, persistent session
Network connection	Network connection
Seperate /home Selected /g/data	Common /home, /scratch and /g/data
No PBS job submission	PBS job submission
Need remote connection to push jobs to Gadi	All jobs can run locally or being pushed to PBS
Suite: Accessdev mode	Suite: Localhost mode Accessdev compatible mode

\$ cat ~/roses/u-da543/suite.rc

```
[runtime]
     [[root]]
     [[] call
         [[[remote]]]
           host = localhost
         [[[dot]]]
            batch system = background
                          Localhost mode
     [[HPC]]
           [remote]]] (host=localhost)
host = localhost
        [[[remote]]]
         [[[dot]]]
           batch system = pbs
       GADI]]
         [[[remote]]]
           host = gadi Accesdev compatible mode
                        (host=gadi,gadi.nci.org.au,.
         [[[dot]]]
            batch system = pbs
```

Connection between ROSE_ORIG_HOST and metascheduler

- Suite localhost mode: No remote connections.
- Suite accessdev mode: Connection between Gadi (gadi.nci.org.au) from \$ROSE_ORIG_HOST
 - ISSUE: Gadi login node, VDI and persistent session can not connect to Gadi (gadi.nci.org.au)
 - SOLUTION: We produced specific ssh config to enable connections within rose/cylc/fcm.
 - Persistent session ==> Gadi (gadi.nci.org.au) utilises the existing ssh key.
 - Gadi login node & VDI ==> Gadi (gadi.nci.org.au) needs to create the ssh key pair (via an initialisation step).

All settings have no impact on user's global ssh environment.

\$ROSE_ORIG_HOST	Localhost Mode	Accessdev Compatible Mode
ARE VDI Gadi Login Node	No remote host detection	Connection from VDI/Gadi login nodes to Gadi (gadi.nci.org.au) requires a specific SSH key pair produced by an initialization script
Persistent Session	No remote host detection	Connection from persistent session to Gadi (gadi.nci.org.au) utilises the existing SSH key pair

Localhost mode is highly recommended in Gadi.

Cylc 8 Platforms

\$ cat ~/roses/u-cz535/flow.cylc

```
[runtime]
  [[root]]
  ...
  [[local]]
    inherit = root
    platform = localhost
  [[HPC]]
    inherit = root
    platform = pbs
```

^{*} Some platforms such as gadi, gadi_pbs, gadi_localhost and gadi_background are still supposed in the current cylc 8 module, in order to transition existing Cylc7 suites to Cylc 8. They will deprecated in the future cylc8 modules.

General workflow

- ps auwxff | grep \$USERNAME
- ssh \$CYLC_SESSION "ps auwxff" | grep \$USERNAME

```
login $ ssh -Y workshopdemo.abc111.xy99.ps.gadi.nci.org.au
  demo $ module use /g/data/hr22/modulefiles
  demo $ module load cylc7/23.09
  demo $ moss-auth
  demo $ rosie co u-da543
  demo $ cd ~/roses/u-da543
  demo $ rose suite-run
```

Replace cylc7/23.09 with cylc/8.2.1 if working with Cylc8 suites

You can monitor the workflow progress later from Gadi login nodes, ARE VDI or persistent session.

Hands-on Excise: Make Your Environment Ready for running Cylc in Gadi

Cylc7 Environment: https://github.com/NCI-HPCDI/cylc-workflow/blob/main/cylc7-guide.md

- ROSE_ORIG_HOST=persistent session
- ROSE_ORIG_HOST=gadi login nodes

Cylc8 Environment: https://github.com/NCI-HPCDI/cylc-workflow/blob/main/cylc8-guide.md ROSE_ORIG_HOST= ARE VDI (for both executing and monitoring)

After the excises, your environment will be ready to run both cylc7 and cylc 8 workflows in Gadi.

Advanced Excise: Cylc 7 Working Directories

Default: the whole ~/cylc-run directory is linked to /scratch/\$PROJECT/\$USER/cylc-run

You can change these links in ~/.metomi/rose.conf

Default	Customised
No changes needed.	Add the following configurations into ~/.metomi/rose.conf [rose-suite-run] root-dir=*=/g/data/\$PROJECT/\$USER root-dir{share}=*=/scratch/\$PROJECT/\$USER root-dir{work}=*=/scratch/\$PROJECT/\$USER
<pre>\$ readlink ~/cylc-run/u-da543 /scratch/fp0/jpf777/cylc-run/u-da543</pre>	<pre>\$ readlink ~/cylc-run/u-da543 /g/data/fp0/jpf777/cylc-run/u-da543 \$ readlink ~/cylc-run/u-da543/work /scratch/fp0/jpf777/cylc-run/u-da543/work \$ readlink ~/cylc-run/u-da543/share /scratch/fp0/jpf777/cylc-run/u-da543/share</pre>

Advanced Excise Guide: https://github.com/NCI-HPCDI/cylc-workflow/blob/main/advanced_guide.md

Advanced Excise: Cylc 8 Working Directories

Default: log, share and work are linked to /scratch/\$PROJECT/\$USER Change these settings via ~/.cylc/flow/global.cylc

```
$ cat ~/.cylc/flow/alobal.cylc
#!Jinja2
Finstall
    source dirs = ~/cylc-src, ~/roses
    [[symlink dirs]]
        [[[aadi]]]
            log = /g/data/{{environ['PROJECT']}}/{{environ['USER']}}
            share = /scratch/{{environ['PROJECT']}}/{{environ['USER']}}
            work = /scratch/{{environ['PROJECT']}}/{{environ['USER']}}
        [[[localhost]]]
            log = /g/data/{{environ['PROJECT']}}/{{environ['USER']}}
            share = /scratch/{{environ['PROJECT']}}/{{environ['USER']}}
            work = /scratch/{{environ['PROJECT']}}/{{environ['USER']}}
```

\$ readlink ~/cylc-run/u-cz535/runN/log /a/data/fp0/jpf777/cylc-run/u-cz535/run1/log 🗽 \$ readlink ~/cylc-run/u-cz535/runN/share /scratch/fp0/jpf777/cylc-run/u-cz535/run1/share \$ readlink ~/cylc-run/u-cz535/runN/work /scratch/fp0/jpf777/cylc-run/u-cz535/run1/work

Advanced Excise Guide: https://github.com/NCI-HPCDI/cylc-workflow/blob/main/advanced_guide.md

Advanced Excise: User Script with Remote Connections

Most remote connections may be unnecessary; consider removing them.

If you still require these remote connections, please add the following configurations to ~/.ssh/config

```
Host gadi.nci.org.au
   Match exec "echo '%l' | grep -q 'ps.gadi.nci.org.au'" host gadi.nci.org.au,localhost
        HostName localhost
   IdentityFile ~/.persistent-sessions/%l/user.key
   StrictHostKeyChecking no
   Port 2222
```

Excise: remove "#" from the following line in ~/roses/u-da543/suite.rc and run the suite again after adding the above configurations to ~/.ssh/config

```
# scp -r STREAM gadi.nci.org.au:~/
```

Possible risks of encountering conflicts in other work.

Advanced Excise Guide: https://github.com/NCI-HPCDI/cylc-workflow/blob/main/advanced_guide.md





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One-On-One: Problem Solving

- Breakout Rooms: Rui/Yue/Martin/Dale
- Opus Documentation

https://opus.nci.org.au/display/DAE/UK+Met+Office+Environment+on+NCI

FAQs

- 2 step fcm-make error in localhost mode
- Restart from checkpoint
- Group membership sync
- How to migrate your Cylc7 suites to Cylc8

Share Suite Run Progress

https://opus.nci.org.au/display/DAE/Sharing+Job+Progress+with+Collaborators

- Start Cylc Review Server
- Monitor Job Progress for Collaborators
- Notes on Data Access
- Share Outside Gadi
 - Nirin instance to host the web server
 - /g/data/ accommodates the static HTML directories