Building robust and reproducible workflows with Cylc and Rose

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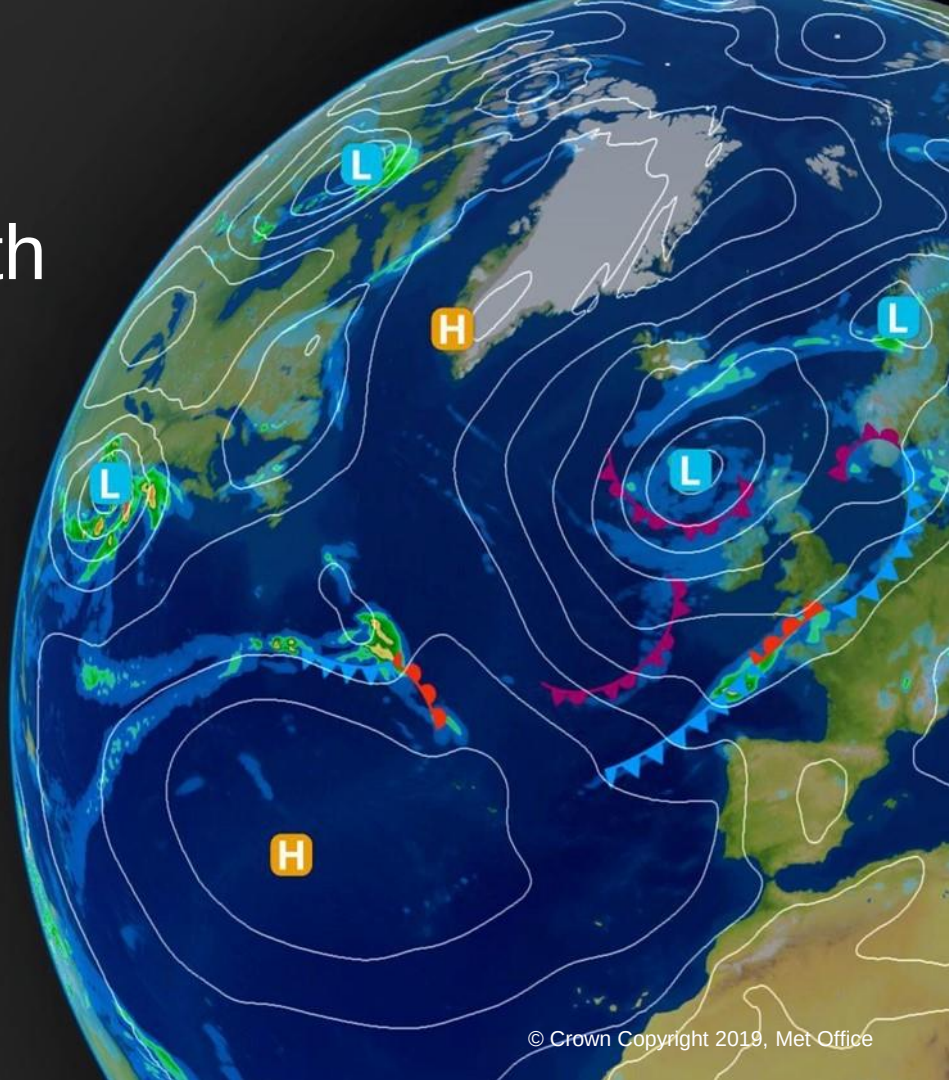

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Introduction to Cylc and Rose

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What is Cylc?

- Cylc is a workflow engine for running suites of inter-dependent jobs
- Cylc can automatically:
  - Submit tasks across computer systems and resource managers.
  - Recover from failures.
  - Repeat workflows.

- Scales to very large, complex workflows
- Cycling suites:
  - Integer, real time, simulated time, externally driven

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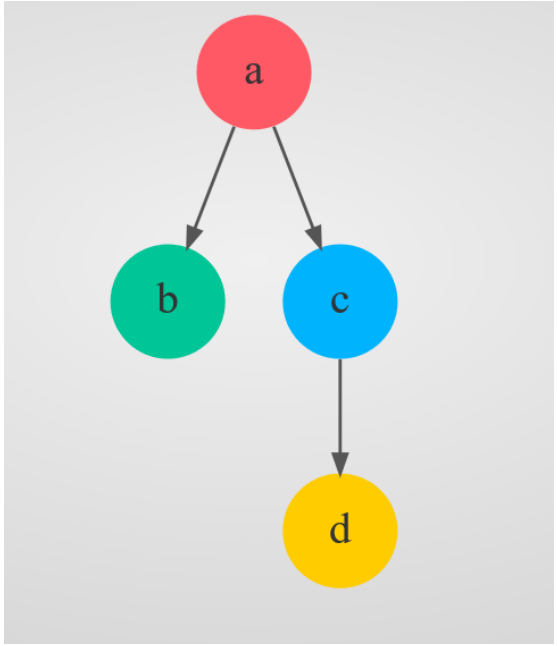
A Simple Workflow



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Simple definition

```
[scheduling]
    [[dependencies]]
        graph = """
            a => c => d
            a => b
"""
```

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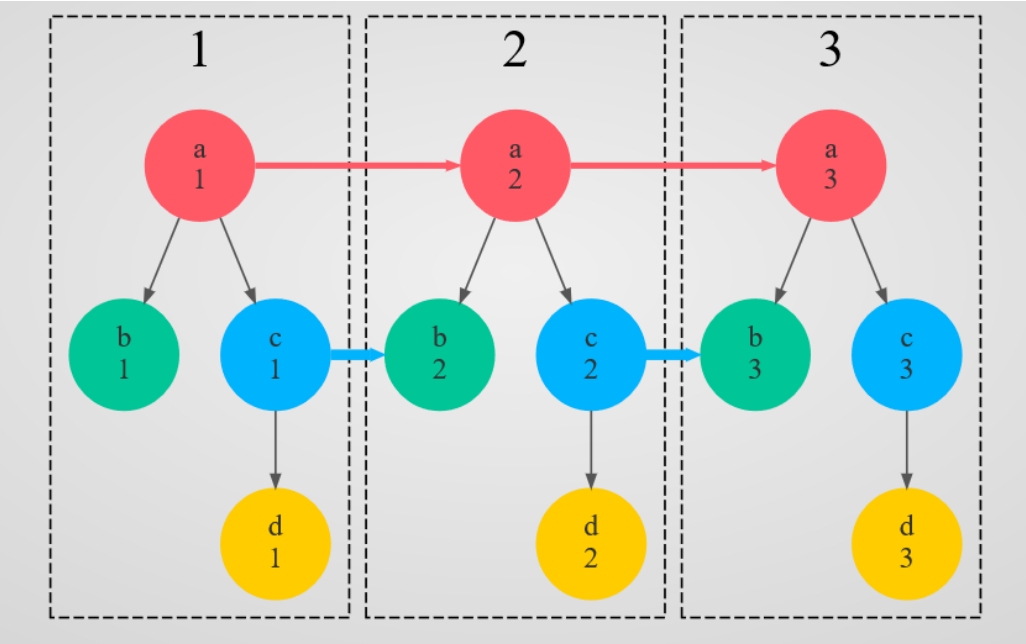
A Repeating Workflow



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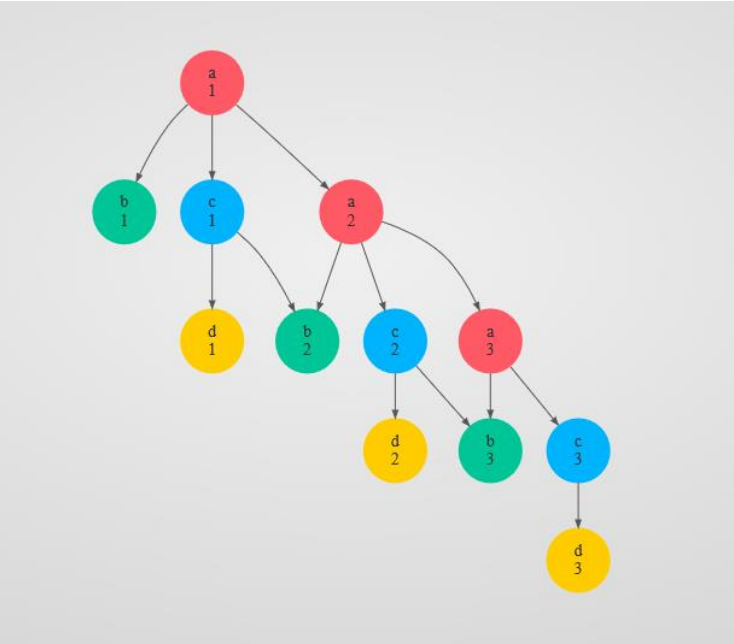
A Cycling Workflow



Cycling definition

```
[scheduling]
    [[dependencies]]
        [[[P1]]]  # Repeat every cycle
            graph = """
                a => c => d
                a => b

                # inter-cycle dependencies
                a[-P1] => a
                c[-P1] => b
"""
```

Date/time cycling

```
[scheduling]
    initial cycle point = 20191014
    final cycle point = 20191016
    [[dependencies]]
        [[[T00,T06,T12,T18]]]
            graph = """
                a => b & c
                a[-PT6H] => a
"""
         [[[T06, T18]]]
             graph = """
                c => x
"""
```

Initial and final dates

Times to run

b and *c* depend on *a*

a depends on *a* from the previous cycle

x depends on *c*, but only for T06 and T18

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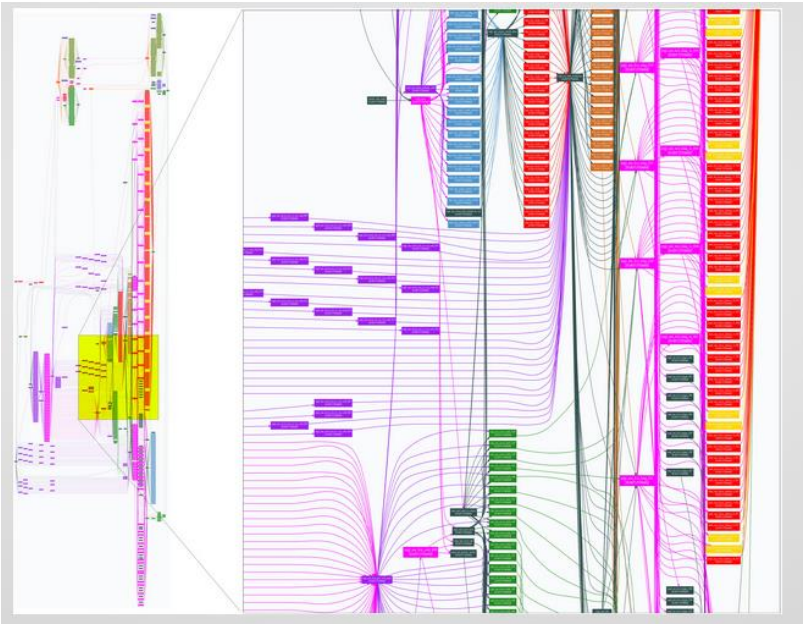
Supports many batch systems

- at
- background
- loadleveler
- lsf
- moab
- pbs
- sge
- slurm

Scaling

- Proven to work at the Met Office with:
  - Thousands of recurrences
  - Tens of thousands of tasks
  - Hundreds of thousands of dependencies

- Met Office workflows are often huge!



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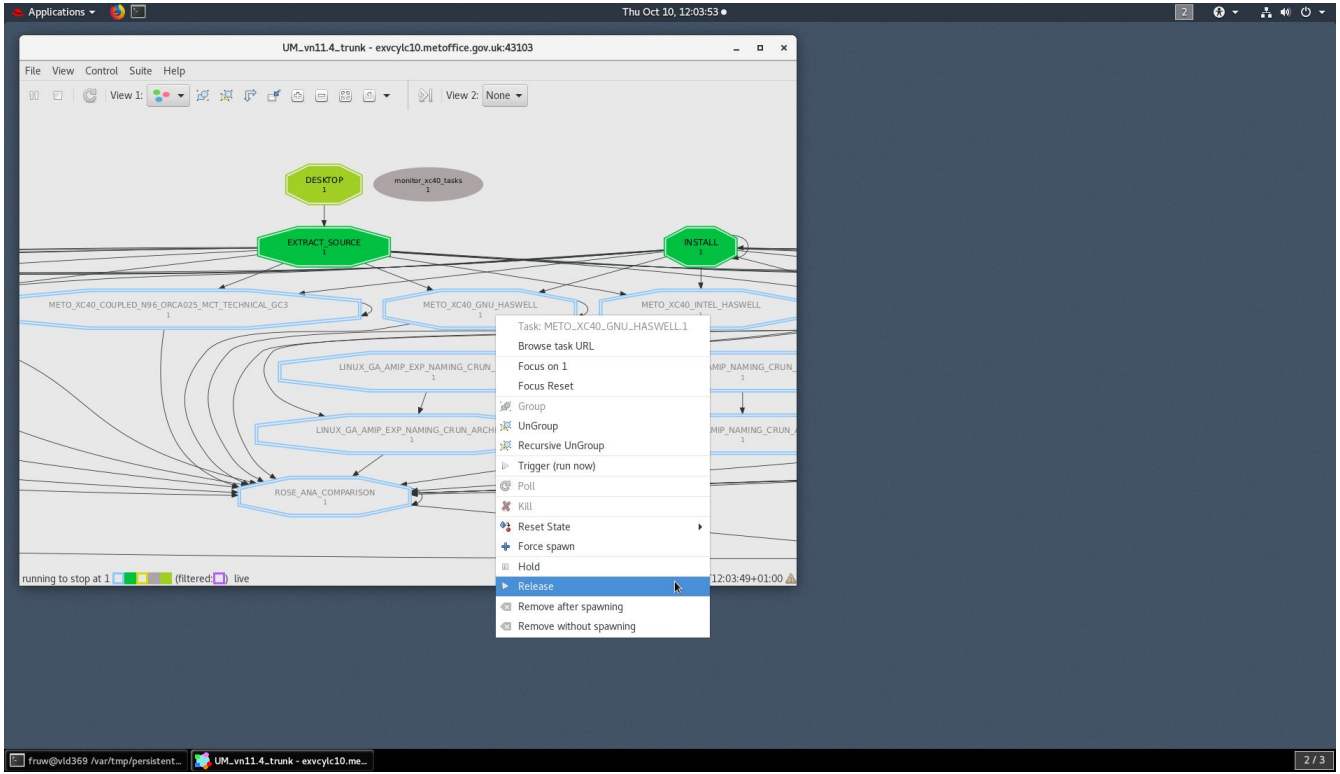
Cylc GUI



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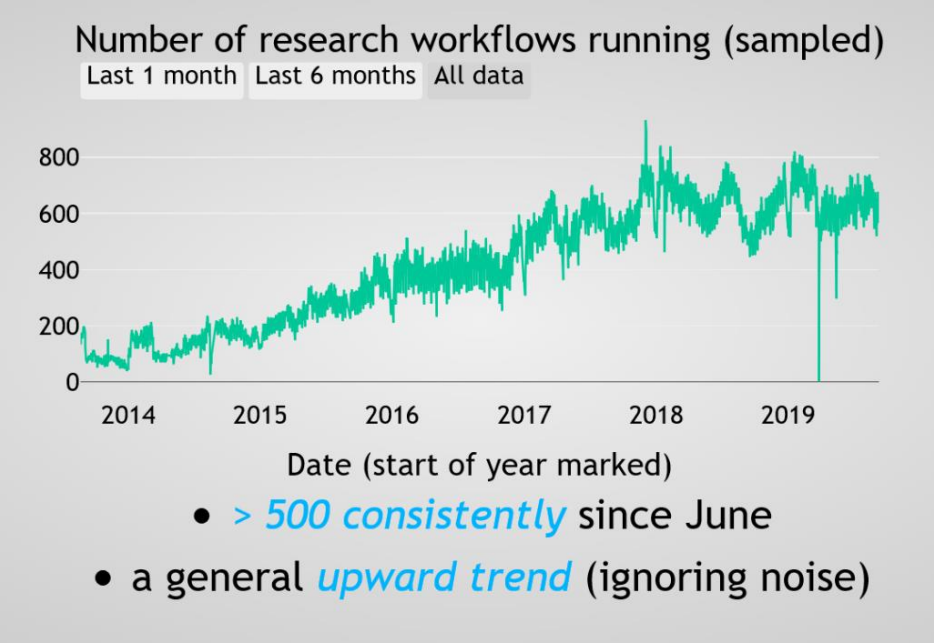
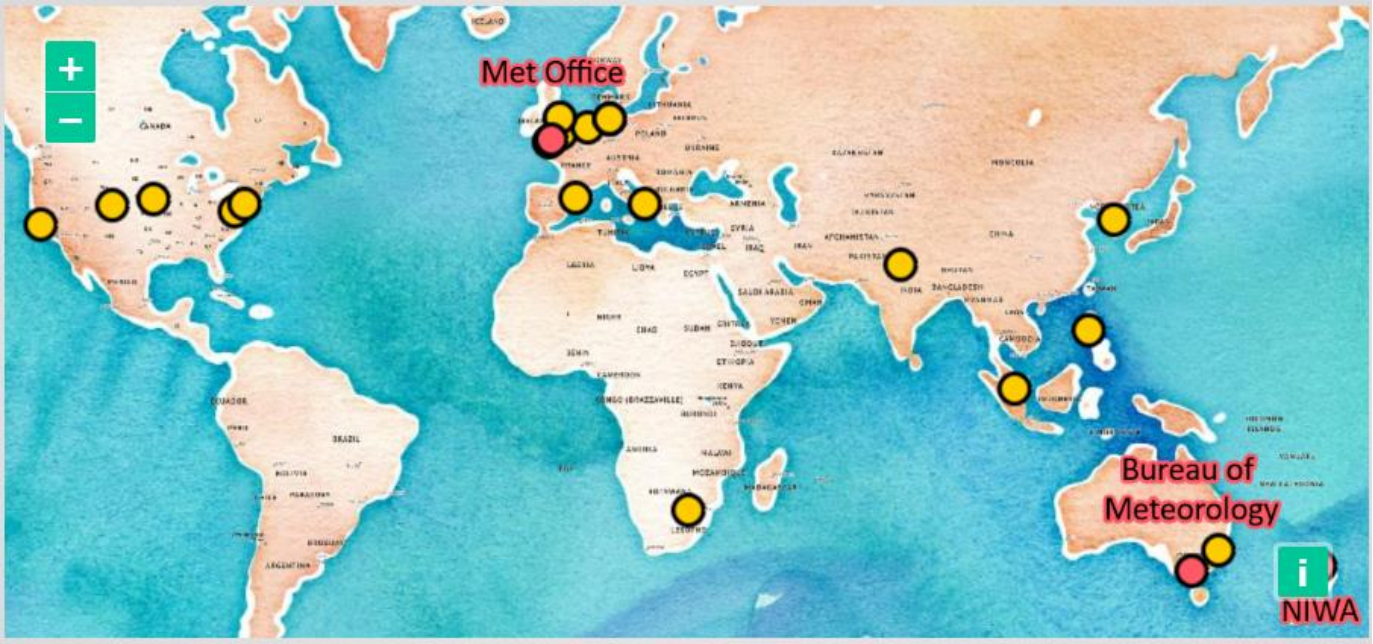
Met Office Usage



Major Sites using Cylc



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What is Rose?

- Rose is a toolkit for writing, editing and running application configurations.

- Rose also contains other optional tools for:
  - Version control.
  - Suite discovery and management.
  - Validating and transforming Rose configurations.
  - Interfacing with Cylc.

Robustness

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Robustness

- How do you ensure that your suite continues to run without manual intervention?
  - E.g. at the weekend, while you're at a conference, on holiday, etc.
- Job fail for a number of reasons
  - With larger and more complex systems there's more chance of a outage
    - E.g. HPC, archive, network problems, etc
    - There are also bugs in code, system errors, etc.
- These can cause errors either in job submission or job execution

Retries

- Cylc can automatically resubmit jobs in the event of failure
- Failures in job submission and job execution can be handled separately
- You can customise the intervals and number of retries

```
[runtime]
    [[atmos]]
        [[[job]]]
            submission retry delays = 3*PT15M
            execution retry delays = 2*PT10M, PT1H
```

ISO8601 durations!

Changing behaviour on retry

```
[runtime]
    [[atmos]]
        script = “””
            test ${CYLC_TASK_TRY_NUMBER} -eq 3
            # do something different
“””
        [[[job]]]
            execution retry delays = PT0S, 2*PT10M
```

Use case:
Changing the timestep when the model fails to converge

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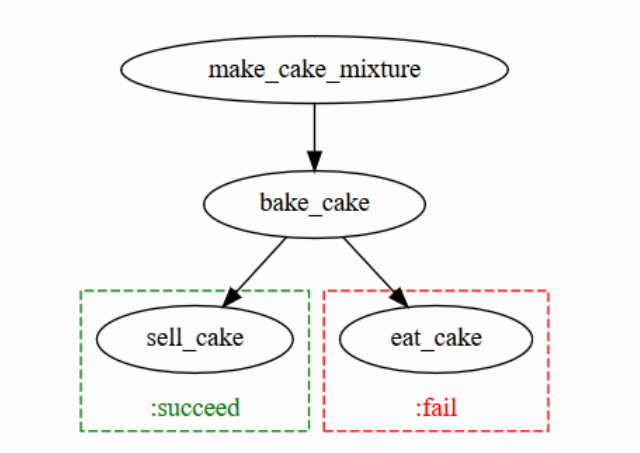
Coping with Failure

- Modify the graph depending on whether a task passed or failed




```
graph = """
make_cake_mixture => bake_cake
bake_cake => sell_cake
bake_cake:fail => eat_cake
"""
```

Changing workflow based on task output

```
[scheduling]
    [[dependencies]]
        graph = “”” arch:archive_success => housekeep
                    arch:archive_fail => other_archive“””
[runtime]
    [[arch]]
        script = “””
            test ${CYLC_TASK_TRY_NUMBER} -eq 3
            # do something different
“””
        [[[job]]]
            execution retry delays = PT0S, PT10M
        [[[outputs]]]
            archive_success = Archiving succeeded
            archive_fail = Archiving failed
```

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Job Polling

- For supported batch systems, polling can query the batch system to determine the job state
- This can be triggered by the user through the GUI…
- … or automatically when a job times out

- Timeouts terminate a job (etc) when Cylc has not heard from the job by an expected time:

```
[[[job]]]
    execution time limit = PT1H
```

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Events and e-mails

- Define a set of events you care about
- If these occur, the system will e-mail you

- Useful if you need to monitor lots of suites, for example:

```
[[[events]]]
    mail events = submission failed, submission retry, failed, retry
```

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Metadata and Validators

- As well as the features in Cylc for runtime robustness, Rose includes validation of the settings in an application.
- For example, ensuring that you're using compatible options

- This is defined by metadata provided by the original developer and tested by the GUI
  - Settings which conflict with the metadata are highlighted
- More complex validation can be done using macros
  - (using Rose's Python API)

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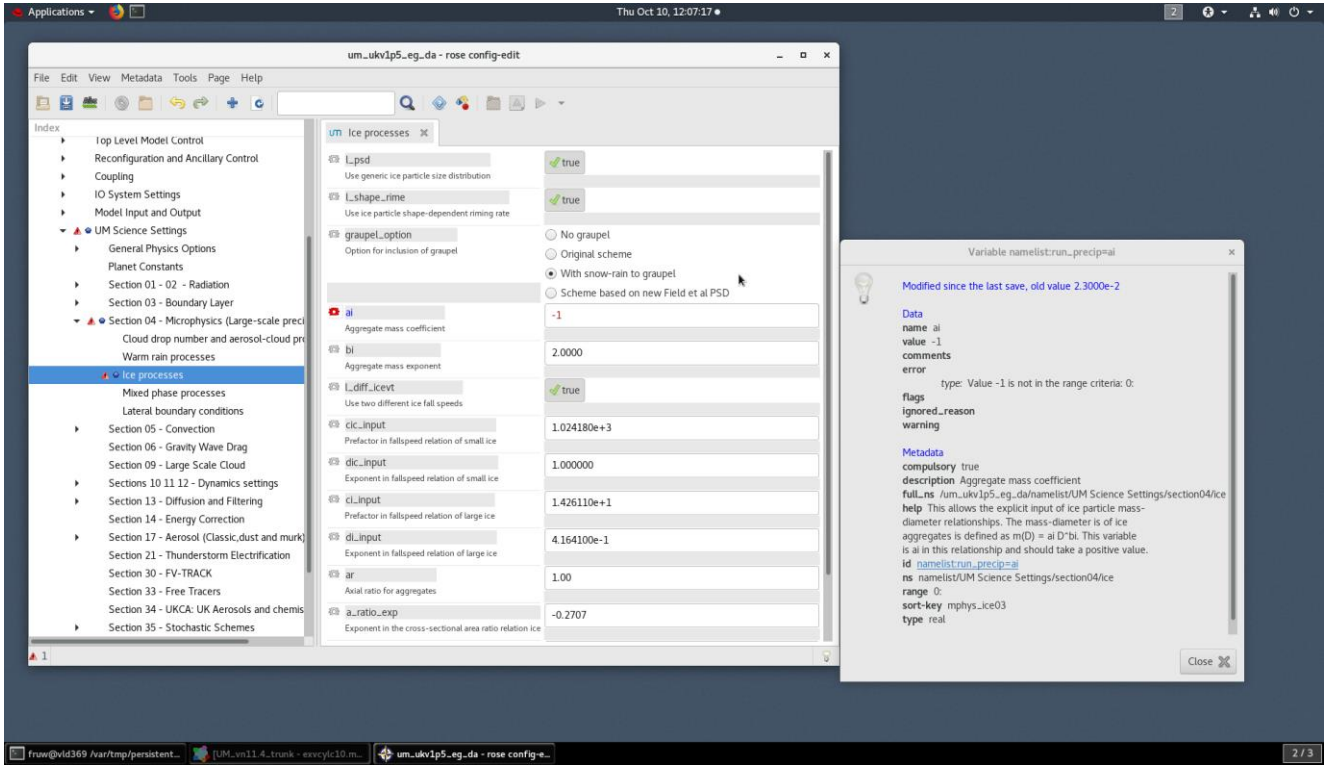
Rose edit GUI



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Reproducibility

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What do we mean by “Reproducible”?

- We run the same tasks in the same order?
  - On a different platform (portability)
- We get bit-comparable results?
- We get scientifically identical results?
- We get the same runtime every time (e.g. no variation in wallclock time)
- We get the same bug every time (e.g. detecting race conditions)

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Reproducing workflows

- Cylc's suite configuration file is a text file, as we've seen
  - No special tools needed so it's easy to edit
- Rose's application configuration file is also a text file
- Version control these files to reproduce the workflow later
  - The whole workflow and configurations inside can be reproduced later
- This doesn't protect from hardware/OS changes!

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Reproducing results

- Getting bit-comparable results is very difficult
  - Eventually you'll be forced to upgrade platforms/compilers which typically change results
  - Often a trade-off between performance/optimisation and getting the same results

- Scientifically identical is more achievable
  - But depends on a scientific judgement as to what is appropriate
  - How good is "good enough"?
  - And this differs depending on the quantity and the application

Conclusion

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Summary

- Cylc and Rose provide a way of creating and reproducing a workflow

- They include lots of functionality to assist in robustness, including:
  - Retries
  - Polling, manual and automatic
  - Failure triggers
  - Events handling
  - Metadata validation

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Where to find out more

- Cylc and Rose are Open Source software
  - Cylc: https://github.com/cylc/cylc-flow
  - Rose: https://github.com/metomi/rose

- Support is available

Questions?

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