JASMIN Workshop: Exercise 7: Manage a multi-step workflow

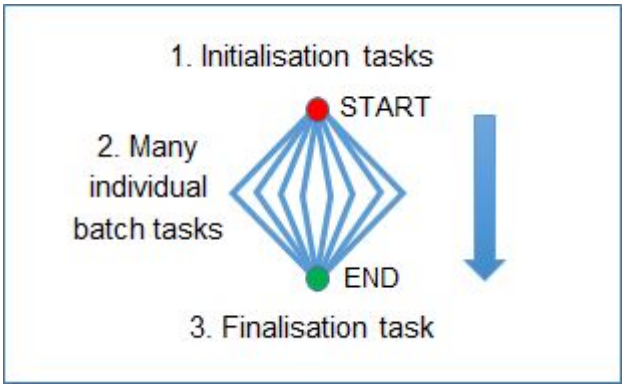
Scenario

I want to analyse a set of historical temperature records from weather stations in the UK. I am interested in calculating annual maximum temperatures for a randomly selected set of 20 counties. These are available from the publicly available "MIDAS-Open" data set in the CEDA archive. There are multiple steps to my workflow so I want to use a tool that (1) can work with LOTUS and (2) can handle dependencies (i.e. only run subsequent tasks if previous tasks have successfully completed).

Objectives

Read data from the MIDAS-Open dataset and aggregate all measurements (from all stations) into a time series of the annual maximum temperatures per county. Then plot a line graph to compare the annual maximum temperature from all counties and write it to a PNG file.

This exercise follows a classic "diamond" structure as follows:



The **(1)** initialisation tasks must be completed first.

The **(2)** individual batch tasks will then all run in parallel.

When they have all completed then the **(3)** finalisation task can be executed.

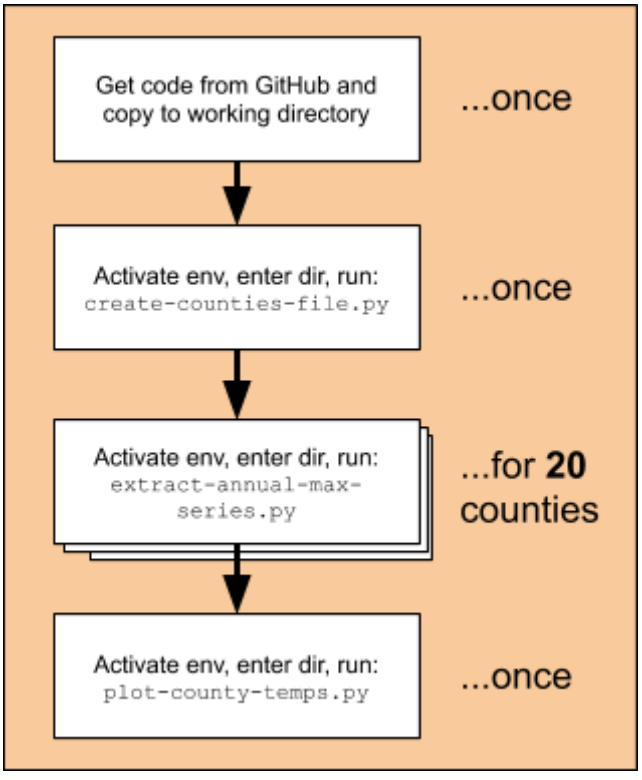
The actual tasks are:

1. **Initialisation**: Clone the repository to get the extraction scripts; run the first script to generate a list of UK counties; write those to a text file.

2. **Batch**: For each county: calculate a 2000-2017 time series of the annual maximum temperature across all stations.

3. **Finalisation**: Read in all the time series files and plot them on a line graph to a PNG file.

It may help to sketch out the process in a simple diagram…as shown here →



An example temperature file for a single station and year (in the MIDAS-Open data set) can be found at:

```
/badc/ukmo-midas-open/data/uk-daily-temperature-obs/dataset-version-201901/devon/01359_cheldon-barton/qc-version-1/midas-open_uk-daily-temperature-obs_dv-201901_devon_01359_cheldon-barton_qcv-1_1977.csv
```

JASMIN resources

- Rose & Cylc (workflow management tools) on the server: `jasmin-cylc.ceda.ac.uk`
- Space to store the output files: in this case they are small so we can write them to the "suite run directory" which lives under the `$HOME` directory
- Access to the Python 3 (Jaspy) environment on JASMIN
- Read-access to the MIDAS-Open data set in the CEDA archive - requires a CEDA account

Local resources

- SSH client (to login to JASMIN)

Instructions

1. Start ssh-agent session and add JASMIN private key
2. SSH to the Rose & Cylc server (with the "`-X`" flag to forward X-windows)
3. In this example you are given the building blocks to construct a "suite file" for use with Rose & Cylc
4. Wrap the scripts in a Rose suite by copying the example suite to a new directory called "`my-suite`" and then modifying it
5. Run the Rose suite
6. If the suite partially runs and leaves log/working directories in place you can clean these up and run it again
7. If you need to stop the suite then you can instruct Cylc to stop it

Review

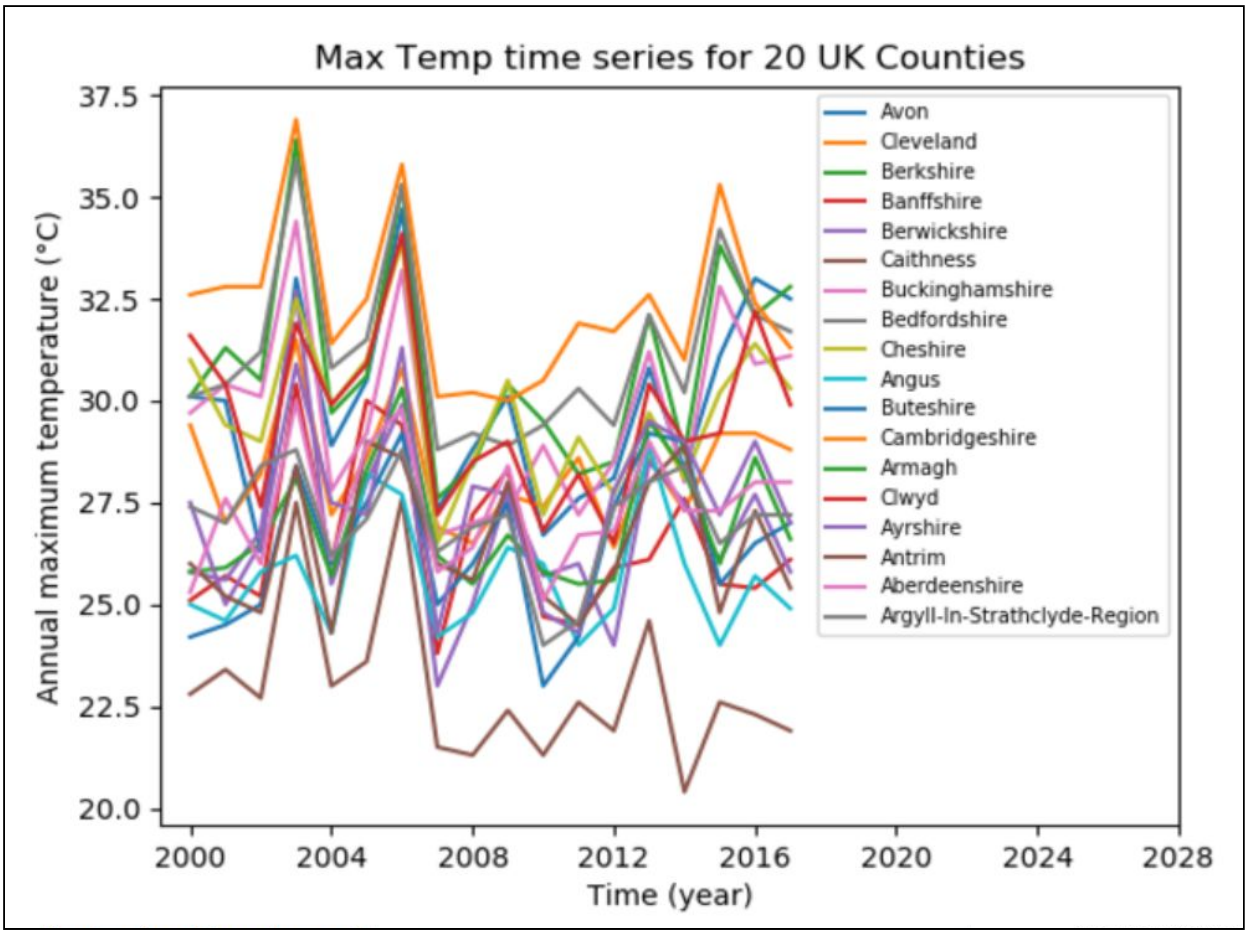
This exercise demonstrates how to:

- Use the Rose and Cylc workflow management tools.
- Construct a Rose suite involving a multi-step workflow.
- Configure a Rose suite to work with the LOTUS batch cluster on JASMIN.
- Run a Rose suite and monitor its progress using the Cylc GUI.

Rose and Cylc are very versatile tools. We recommend that you study the documentation at:

Rose: https://metomi.github.io/rose/doc/html/
Cylc: https://cylc.github.io/doc/built-sphinx/
Cheat sheet: https://metomi.github.io/rose/doc/html/cheat-sheet.html

You should end up with a graph of time series data that looks something like:



Alternative approaches and best practice

- Manage the process yourself (without Rose and Cylc)?
- Set the `$PATH` environment variable in your `~/.bash_profile`
- Write your outputs somewhere else
- *Have any files been accidentally left on the system? /tmp/ etc*
- Tidy up your run suite directory (i.e. logs and task directories)
- View the workflow graph of the suite
- Understand different modes of stopping a running suite

Cheat sheet for Exercise 7: Manage a multi-step workflow

1. Start ssh-agent session and add JASMIN private key (skip if already done)

```
eval $(ssh-agent -s)
ssh-add ~/.ssh/id_rsa_jasmin
```

2. SSH to the Rose & Cylc server (with the "`-X`" flag to forward X-windows)

```
ssh -A -X <username>@jasmin-login1.ceda.ac.uk
ssh -X jasmin-cylc
```

3. In this example you are given the building blocks to construct a "suite file" for use with Rose & Cylc:

    - Script 1: `create-counties-file.py`
        i. Context: Python 3
        ii. Inputs: None - script locates county directories in CEDA Archive
        iii. Outputs:
            1. File: `./outputs/counties.txt`

    - Script 2: `extract-annual-max-series.py`
        i. Context: Python 3
        ii. Inputs: index - to select a county from the list (a number between 1 and 20)
        iii. Outputs:
            1. Files [20]: `./outputs/<county>.csv`

    - Script 3: `plot-county-temps.py`
        i. Context: Python 3
        ii. Inputs: None - script locates input data in the "`./outputs/`" directory
        iii. Outputs:
            1. File: `./outputs/annual-max-temp-time-series.png`

    - The scripts are available in:
      `/group_workspaces/jasmin2/workshop/exercises/ex07/code/`
      And in github at:
      https://github.com/cedadev/jasmin-workshop/tree/master/exercises/ex07/code

4. Wrap the scripts in a Rose suite by copying the example suite to a new directory called "`my-suite`" and modifying it. (Or you can simply use the "`workshop-suite`" already provided).

    - The example suite is available at:
      `/group_workspaces/jasmin2/workshop/exercises/ex07/example-suite`

    - Go to the directory where you have copied the suite.

    - You can run the example suite to view how it works, with:

```
# Add the location of the rose/cylc executables to $PATH
export PATH=/apps/contrib/metomi/bin:$PATH
rose suite-run
```

- All of the scripts operate on input/output data in the relative directory: "`./outputs`". It therefore makes sense to copy the Python scripts to the main suite "run directory" and ensure that each task runs from that directory. The suite run directory is specified by the Cylc environment variable: `$CYLC_SUITE_RUN_DIR`.

- Edit the "`suite.rc`" file as follows:
  i. In the "`[[runtime]]`" section of the suite file, modify each of the 4 processing steps as follows:

1. `[[initialise]]`
   a. Clone the GitHub repository: https://github.com/cedadev/jasmin-workshop
   b. Copy the files in the sub-directory "`jasmin-workshop/exercises/ex07/code/`" to the suite run directory at: `$CYLC_SUITE_RUN_DIR`

2. `[[step1]]`
   a. Activate the standard JASMIN Python 3 environment.
   b. Change directory to `$CYLC_SUITE_RUN_DIR`
   c. Run the script

3. `[[batch<counter>]]`
   a. Activate the standard JASMIN Python 3 environment.
   b. Change directory to `$CYLC_SUITE_RUN_DIR`
   c. Run the script for each value of the "`counter`":
      i. The "`counter`" variable is accessible by the environment variable:
      `$CYLC_TASK_PARAM_counter`

4. `[[final]]`
   a. Activate the standard JASMIN Python 3 environment.
   b. Change directory to `$CYLC_SUITE_RUN_DIR`
   c. Run the script

5. Run the Rose suite with the command:

```
export PATH=/apps/contrib/metomi/bin:$PATH
rose suite-run
```

   - **NOTE:** It will take a couple of minutes to start up and then a GUI should appear that shows the workflow in action.

6. If the suite partially runs and leaves log/working directories in place you can clean these up and run it again with:

```
rose suite-run --new
```

7. If you need to stop the suite you can use:

```
cylc stop '<SUITE>'
# Where <SUITE> is the name of the suite directory, such as "my-suite"
```

What does the Cylc GUI look like?

Here is a quick walk-through of what you should see in the GUI if the job runs successfully. Note that in this example the 4 tasks have been renamed to:

- `clone_repo`
- `get_counties`
- `process<county>`
- `plot`

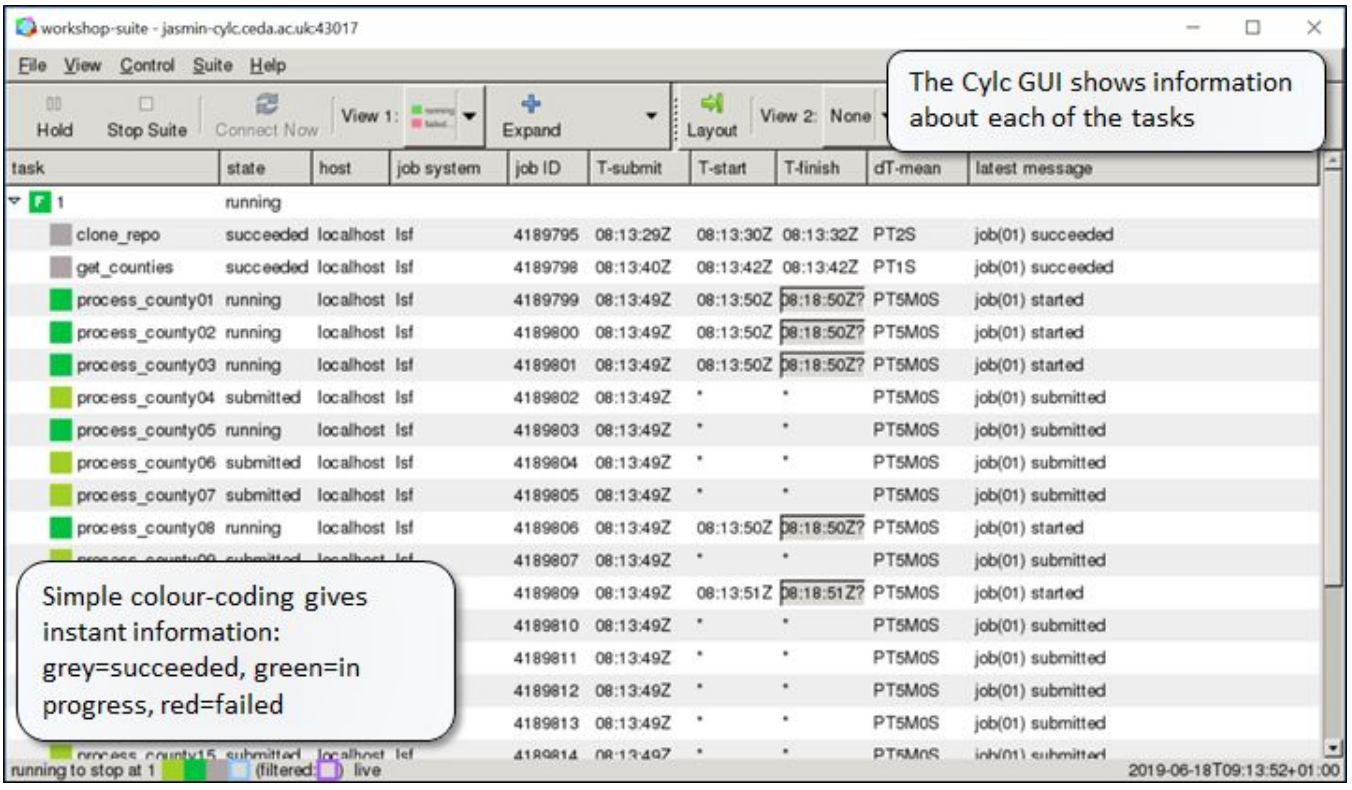
The full example suite is available at:

`/group_workspaces/jasmin2/workshop/exercises/ex07/workshop-suite`

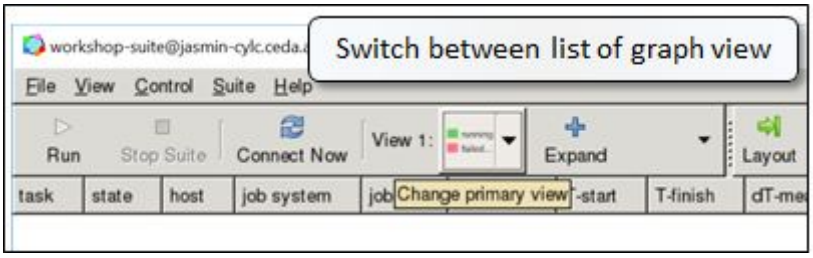
And in github at:

https://github.com/cedadev/jasmin-workshop/tree/master/exercises/ex07/workshop-suite

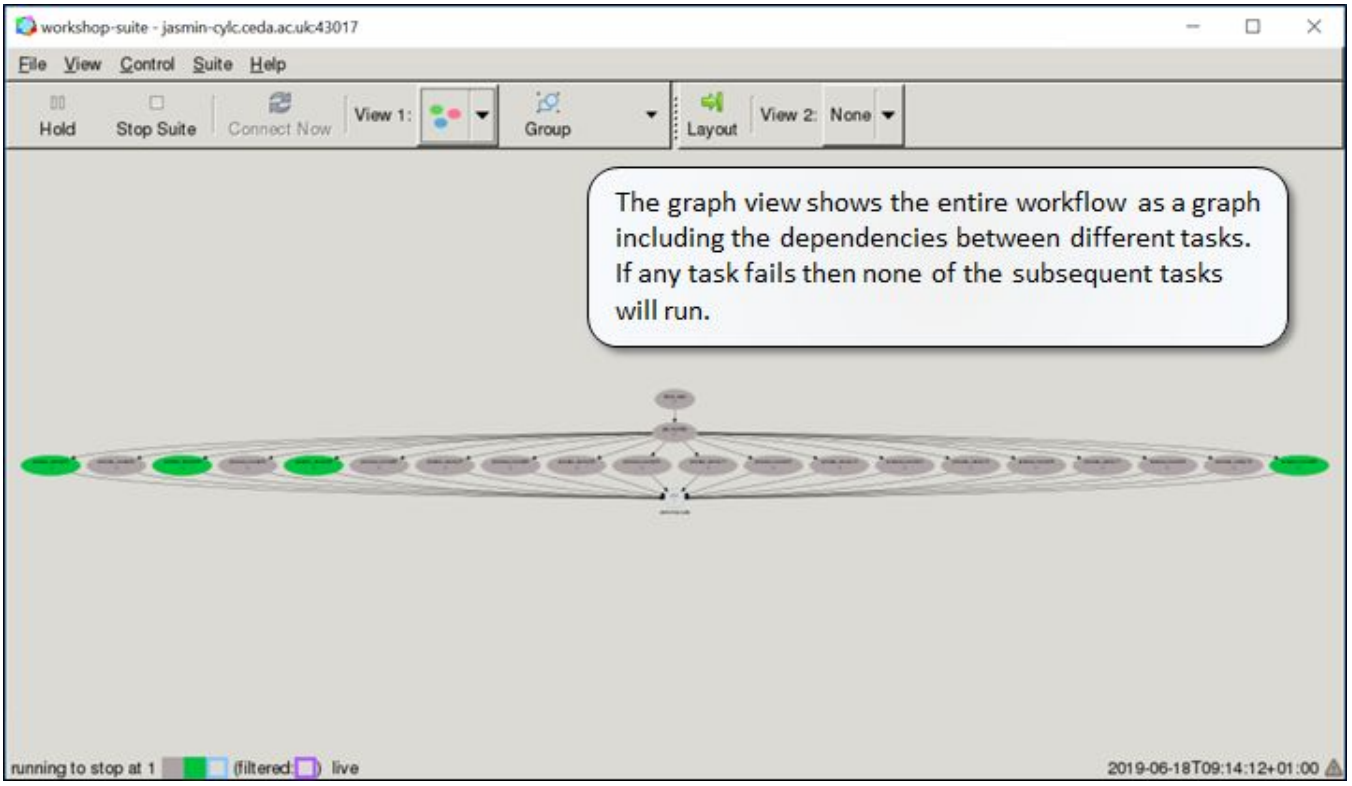
The Cylc GUI opens when you start running a suite (as long as you have used the "`-X`" flag when SSHing to the server).



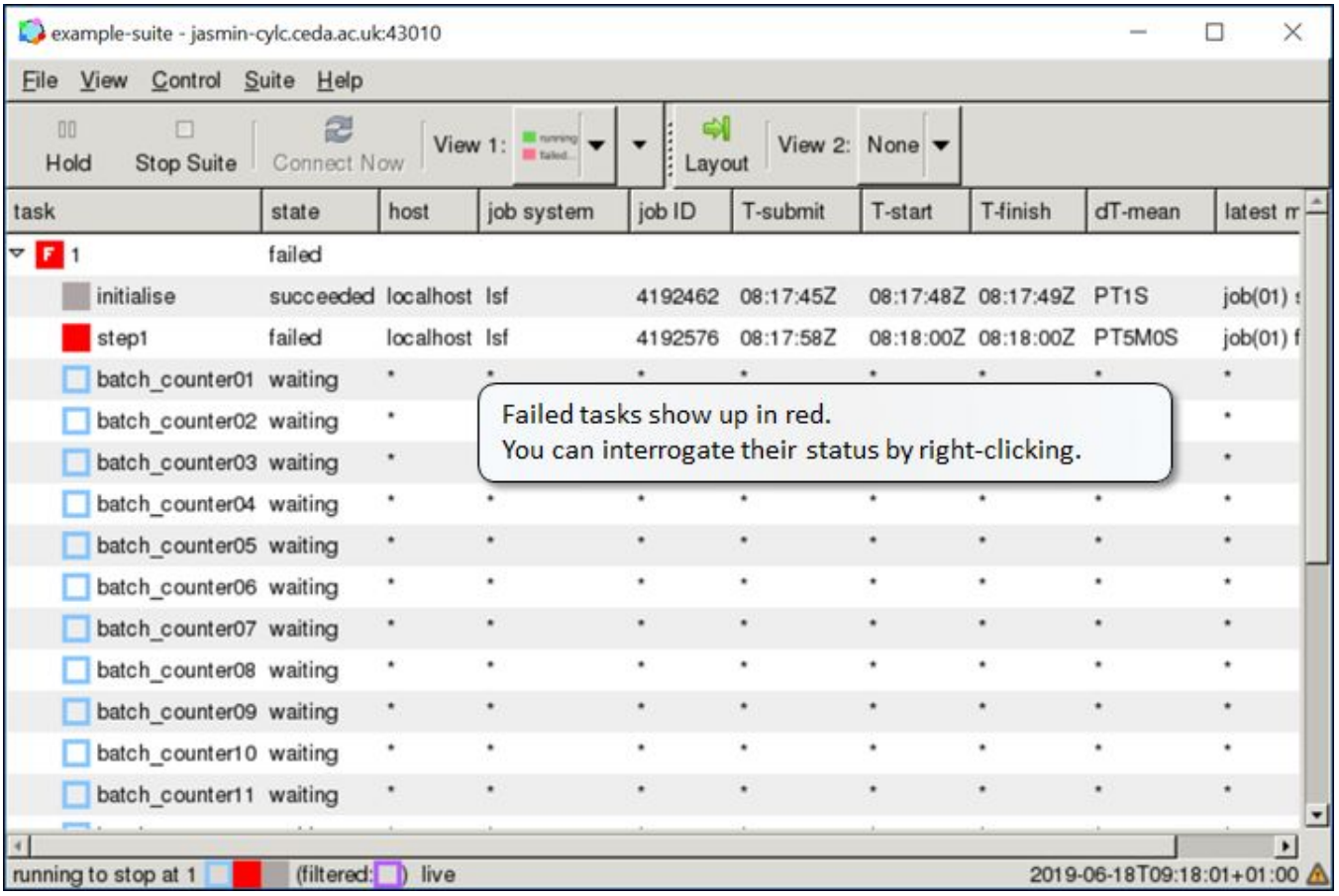
You can select either a list view (as above) or a graph view (below) of the workflow.



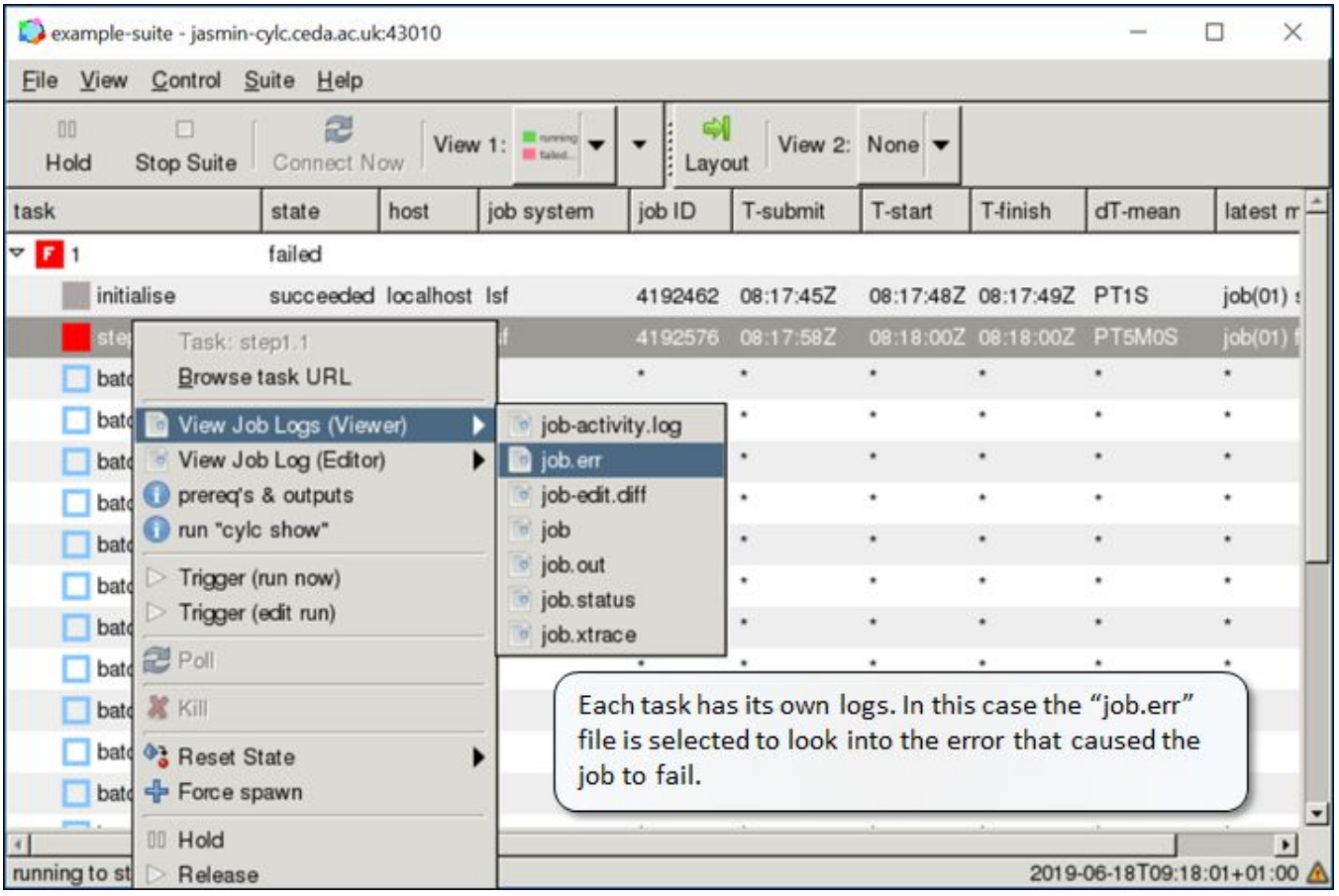
The graph view shows each of the tasks and the dependency graph that connects them.



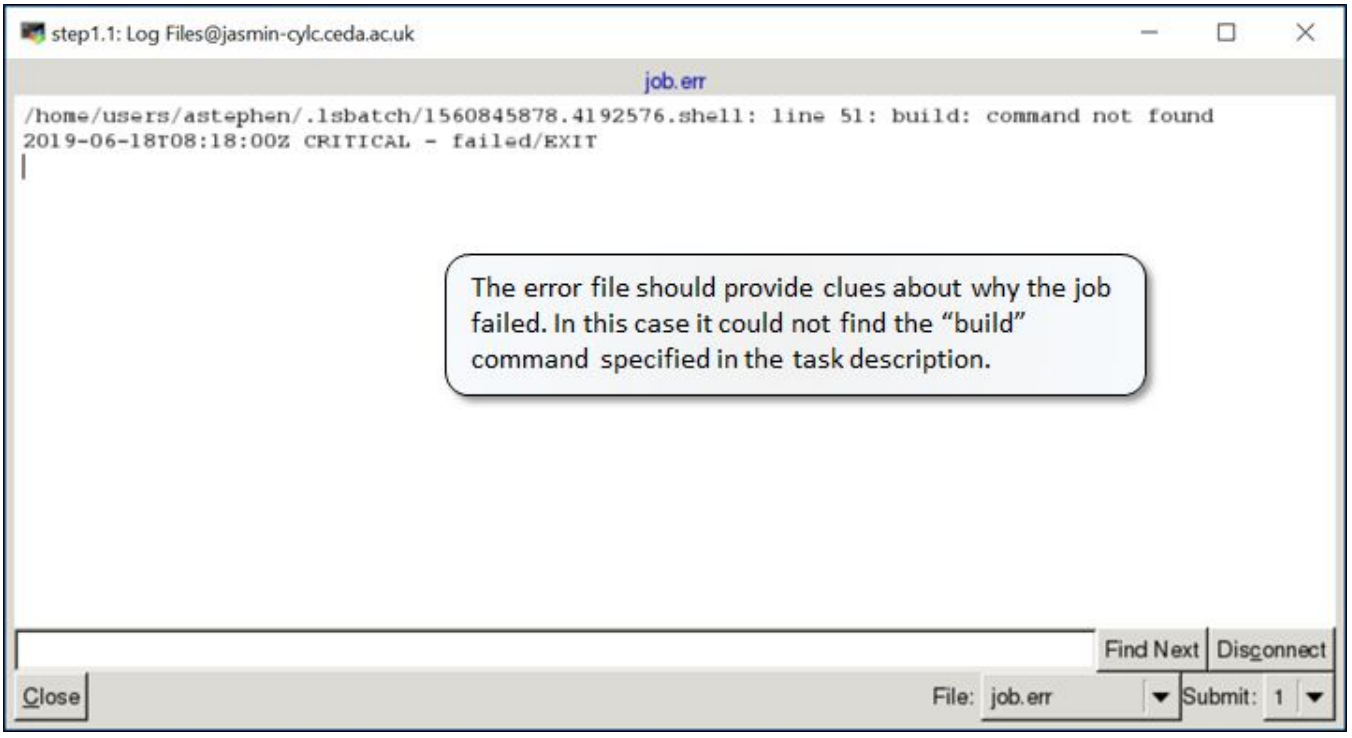
Failed tasks are clearly indicated in red.



Right-click on a failed task in order to view more information.



Each of the log files can be viewed within the GUI.



Alternative approaches and best practice

- Manage the process yourself (without Rose and Cylc):
  - Pros:
    - You don't need to learn how to configure Rose and Cylc
  - Cons:
    - You have to check the dependency tree yourself:
      - You need to check whether all tasks have run in a given stage before progressing to the next stage.
    - With Rose and Cylc you can configure complex rules for responding to failures and retrying tasks.

- Write your outputs somewhere else:
  - You might write outputs directly to a Group Workspace
  - You might write outputs to the default working directory for a task:
    - These are symbolically linked to the global "`/work/scratch/$USER`" area.
  - See more details in the Rose documentation: https://metomi.github.io/rose/2019.01.0/html/tutorial/cylc/runtime/introduction.html#where-do-all-the-files-go

- Set the `$PATH` environment variable in your `~/.bash_profile`
  - In order to find the Rose/Cylc variables we needed to change the `$PATH` as follows:

```
# Add the location of the rose/cylc executables to $PATH
export PATH=/apps/contrib/metomi/bin:$PATH
```

  - You can put the following lines in your "`~/.bash_profile`" file so that this will happen automatically when you login to the `jasmin-cylc` server:

```
if [[ $HOST = "jasmin-cylc.ceda.ac.uk" ]]; then
    export PATH=/apps/contrib/metomi/bin:$PATH
fi
```

- *Have any files been accidentally left on the system? /tmp/ etc*
  - Running a Rose suite will copy your suite to a "run suite directory" under:
    - `$HOME/cylc-run/<SUITE>/`
  - This directory includes various files, directories and symbolic links related to your job. Please check that you are not writing big files to that the directory and monitor the size of the outputs.

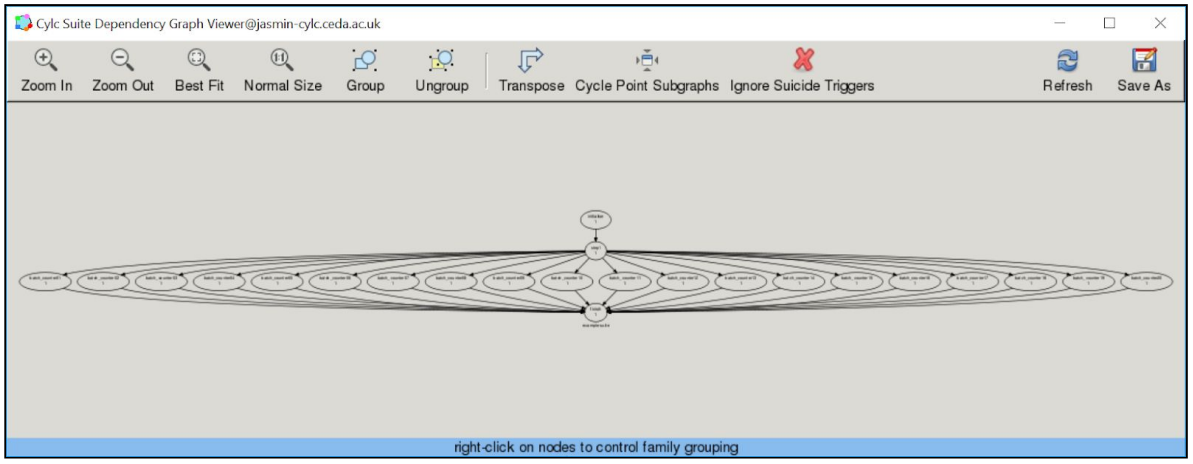
- Tidy up your "run suite directory" (i.e. logs and task directories):
  - You can instruct Rose to tidy up (clear out) any logs and task directories by using the command:

```
rose suite-clean
```

- View the workflow graph of the suite:
  - To view the workflow graph of your suite *without* running it, use:

```
rose suite-run -i
cylc graph '<SUITE>'
# Where <SUITE> is the name of the suite directory
```

  - NOTE: the "`-i`" option means "install only" - so this will not run the suite.



- Understand different modes of stopping a running suite:
  - If you need to stop a suite that is running you can use:

```
cylc stop '<SUITE>'
# Where <SUITE> is the name of the suite directory
```

  - To restart a STOPPED suite:

```
cylc restart '<SUITE>'
# Where <SUITE> is the name of the suite directory
```

  - The `cylc stop` command may not stop the suite immediately - because it will wait for submitted and running tasks to complete. To kill the submitted and running tasks before stopping the suite, use:

```
cylc stop --kill '<SUITE>'
```

  - To stop the suite regardless of submitted and running tasks, use:

```
cylc stop --now '<SUITE>'
```