

NCAS Unified Model Introduction: Practical sessions (Rose/Cylc)

NCAS-CMS

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Can also be used for self-study.

NCAS Computational Modelling Services: http://cms.ncas.ac.uk/

SECTION

ONE

GETTING SET UP (SELF-STUDY INSTRUCTIONS)

Warning: You **MUST** have PUMA2, ARCHER2 and MOSRS accounts setup before starting this section.

Warning: If you have moved your account over to PUMA2 from the old PUMA server (pumanew), then you should follow these instructions: https://cms.ncas.ac.uk/puma2/

1.1 Set up your ARCHER2 connection

To use the UM Introduction Tutorials you will first need to ensure you can connect from your local desktop to ARCHER2. There a multiple ways in which you can do this depending on your desktop platform:

- via Terminal on GNU/Linux & macOS
- via MobaXTerm on Windows

1.1.1 SSH key files

Before you try and connect to ARCHER2, you need to make sure that you have the ssh-keys available on your computer. In these instructions, we've assumed the keys are called id_rsa_archer2 and id_rsa_archer2.pub. Replace with the name of your keys as appropriate.

1.1.2 Connecting via a Terminal (GNU/Linux & macOS)

It is possible to connect via a terminal with an X11 connection (XQuartz is also required when using macOS) Login to ARCHER2:

```
ssh -Y -i ~/.ssh/id_rsa_archer2 <archer2-username>@login.archer2.ac.uk
```

To simplify the login process, you can define a \sim /.ssh/config file entry containing the necessary information. For example:

```
Host archer2
Hostname login.archer2.ac.uk
User <archer2_username>
IdentityFile ~/.ssh/id_rsa_archer2
```

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```
ForwardX11 yes
ForwardX11Trusted yes
```

so that you can connect using just the command:

```
ssh archer2
```

1.1.3 Connecting via MobaXTerm

- From Chrome, go to page: https://mobaxterm.mobatek.net/download.html
- Under "Home Edition" select "Download now"
- On next page select "MobaXterm Home Edition v23.4 (Portable edition)". This should download the package.
- Click the download icon in the bottom left hand corner.
- Double-click on the **MobaXterm_Personal_23.4** application file, and select "Extract all". A new directory window will open up.
- Double-click **MobaXterm_Personal_23.4** to launch the application.

Next time, navigate to "Downloads" to open the application.

1.2 Set up your ARCHER2 environment

Login to ARCHER2 from your local desktop, copy the following profile to your home directory.

```
archer2$ cp /work/y07/shared/umshared/um-training/rose-profile ~/.profile
```

Change the permissions on your /home and /work directories to enable the NCAS-CMS team to help with any queries:

```
chmod -R g+rX /home/n02/n02/<your-username>
chmod -R g+rX /work/n02/n02/<your-username>
```

1.3 Set up your PUMA2 connection

PUMA2 is accessed from the ARCHER2 login nodes, and you will use the same username and password.

From an ARCHER2 terminal type:

```
archer2$ ssh -Y puma2
```

and type your ARCHER2 password when prompted.

You should now be logged into PUMA2. To go back to the ARCHER2 login nodes, type exit.

1.3.1 Set up passwordless access to PUMA2

You can set up a passphrase-less ssh-key to allow you to connect to PUMA2 without typing a password or passphrase.

Note: We would never normally advise using an ssh-key without a passphrase, but in this case it is safe to do so since we are already authenticated within the ARCHER2 system.

From the ARCHER2 login nodes, type:

```
archer2$ ssh-keygen -t rsa -f ~/.ssh/id_rsa_puma2
```

At the prompt, press enter for an empty passphrase.

Copy the key over to PUMA2:

```
archer2$ ssh-copy-id -i ~/.ssh/id_rsa_puma2 puma2
```

Type in your ARCHER2 password when prompted.

Next, create a file called ~/.ssh/config (if it doesn't already exist), and add the following lines:

```
Host puma2
IdentityFile ~/.ssh/id_rsa_puma2
ForwardX11 yes
```

Test it works by typing:

```
archer2$ ssh puma2
```

You should not be prompted for your password. Note that this should have set up X11 forwarding, so you no longer need the -Y option.

Warning: You should never use a passphrase-less key to access the ARCHER2 login nodes, as this is a serious security risk.

1.4 Set up your PUMA2 environment

Copy our standard .profile and .bashrc files:

```
puma2$ cd
puma2$ cp ~um1/um-training/puma2/.bash_profile .
puma2$ cp ~um1/um-training/puma2/.bashrc .
```

Logout of PUMA2 and back in again to pick up these changes.

You will get a warning about not being able to find ~/.ssh/ssh-setup. This can be ignored and will be resolved in the next step.

You should also be prompted for your Met Office Science Repository Service password, then username. Note that it asks for your **password** first. Remember your MOSRS username is one word; usually firstname-lastname, all in lowercase.

If the password caching works, you should see:

Subversion password cached Rosie password cached

This means you can now access the code and roses suites stored in the Met Office respositories.

Note: The cached password is configured to expire after 12 hours. Simply run the command mosrs-cache-password to re-cache it if this happens. Also if you know you won't need access to the repositories during a login session then just press return when asked for your MOSRS password.

Finally, change the permission on your PUMA2 /home space:

```
chmod -R g+rX /home/n02/n02/<your-username>
```

1.5 Set up your ssh-agent

In order to submit jobs to ARCHER2 from PUMA2, you will need to set up an ssh-agent and use it to cache the passphrase to your ARCHER2 key.

i. Copy your ARCHER2 ssh-key pair to PUMA2

Your ARCHER2 key is the one that you use to ssh into the ARCHER2 login nodes. You need to copy both the public and private keys into your .ssh/directory on PUMA2.

Open a new terminal from wherever you originally connected to ARCHER2 in *Set up your ARCHER2 connection*, and run the following command

ii. Start up your ssh-agent

First copy the ssh-setup script to your .ssh/directory.

```
puma2$ cp ~um1/um-training/setup/ssh-setup ~/.ssh
```

Next log out of PUMA2 and back in again to start up the ssh-agent process. You should see the following message

```
Initialising new SSH agent...
```

iii. Add your ARCHER2 key

Add your ARCHER2 key to the ssh-agent, by running

```
puma2$ ssh-add ~/.ssh/id_rsa_archer2
```

Enter your passphrase when prompted. If the passphrase has been cached successfully you should see a message like this:

```
Identity added: /home/n02/n02/<archer2-username>/.ssh/id rsa archer2
```

The ssh-agent will continue to run even when you log out of PUMA2. However, it may stop from time to time, for example if PUMA2 is rebooted. For instructions on what to do in this situation see *Restarting your ssh agent* in the Appendix.

iv. Configure access to the ARCHER2 login nodes

Create a file ~/.ssh/config (if it doesn't already exist), and add the following lines:

```
# ARCHER2 login nodes
Host ln*
IdentityFile ~/.ssh/id_rsa_archer2
```

iv. Verify the setup is correct

To test this is all working correctly, run:

```
puma2$ rose host-select archer2
```

This should return one of the login nodes, e.g. ln01. If it returns a message like [WARN] ln03: (ssh failed) then something has gone wrong with the ssh setup.

You are now ready to try running a UM suite!

WORKING WITH SUITES

2.1 Suite Discovery and Management: rosie go

Rosie go is the suite manager GUI. It acts as a hub for all your suite work. From rosie go it is possible to search for suites, create, checkout, delete, edit, run suites and more. We will take a look at the main features here.

Launch rosie go by typing:

puma2\$ rosie go

2.1.1 Searching for suites

By default, rosie go will show all the suites that you have checked out locally, so unless you have used Rose before you will have an empty results panel to begin with. You can search for suites by typing a word/phrase into the *Search* box and either click the *Search* button or press <Enter>. The search looks for the entered word/phrase in **any** of a suite's properties.

• Enter **u-ag137** in the *Search* box and press <Enter>

You should now see a long list of suites. All these suites are listed as they reference u-ag137 in their suite information.

More advanced queries can be run by clicking the + button next to the Search button. Queries allow you to filter results based on the values of particular properties. You can combine filters to make complex queries.

• Select **idx** in the property box and **eq** in the operator box and then enter the value **u-ag137**. Click *Query*.

This time you should only see one suite listed in the results pane.

• Now run a query to list all suites owned by rosalynhatcher containing ARCHER2 in their title.

The searches you run within rosie go are recorded in your search history.

• View your history by clicking *History -> Show search history*.

The *Search History* panel should now be displayed on the left-hand side of rosie go listing your past searches. You can order the results by type, parameters or whether you asked to see all revisions by clicking on the relevent column head. To re-run one of these searches simply click on it.

• Try running your initial search for u-aq137 again.

Close the Search History Panel by clicking the close button (X) in the top-right of the panel.

2.1.2 Viewing suite information

To obtain more information about a suite listed in the search results you can do one of two things:

- 1. Hold your mouse over the suite to display a tooltip containing more details
- 2. Right click on the suite and select *Info* in the pop-up menu to display a dialog box containing further details
- What project is suite u-ab878 associated with?

Suite search results can be ordered by property in either ascending or descending order. To do so, click on the column title for the property you wish to order by so an arrow is displayed next to it indicating the order in which the property is being sorted.

2.1.3 Checking out an existing suite

Right-clicking on a suite displays a pop-up menu from which you can perform many functions on the suite; e.g. checkout, copy, delete, run, etc. We will perform many of these actions in subsequent exercises but to begin with we will just checkout an existing suite to use in the *Editing Suites: rose edit* exercises. To view a suite it must be checked out first.

• Right-click on suite u-ag137 and select *Checkout Suite* from the pop-up menu.

When you checkout a suite it is always placed in your ~/roses directory. In this state, the suite is simply a working copy - you can edit it and run it but any changes you make will only be held locally.

Note: You can also checkout a suite by highlighting it and then clicking the *Checkout* button on the toolbar or by running rosie checkout <suiteid> on the puma2 command-line.

2.1.4 Other useful features

To see what suites you have checked out click the *Show local suites* button to the left of the search box (represented by the *house* icon). You should have at least 1 suite listed.

• What do you think the *house* icon in the local column indicates?

2.2 Editing Suites: rose edit

The rose config editor in combination with the metadata file, which describes UM inputs, is the GUI for editing UM suites. Building and running the UM under Rose requires, at least, two separate apps: an fcm_make app to build the model executable and a um app to configure the runtime namelists and environment variables. Coupled models may require additional fcm_make apps, one for each executable to be built.

2.2.1 Launch the config editor GUI

Right click on suite u-ag137 and select *Edit Suite*. The rose edit GUI will start up.

On the left hand side is a navigation panel containing a tree listing the apps in the suite. For this particular suite these are:

- suite conf General suite configuration options
- fcm_make_pp Extract and build the post-processing scripts
- fcm make um Extract and build the UM source code
- housekeeping Tidies up log files, old work and data directories
- install_ancil Install ancillary files
- postproc Post-processing settings
- rose_ana Rose built in app; used here for comparison of dump files
- rose_arch Rose built in app; used here for archiving of log files
- um The UM atmosphere and reconfiguration settings

2.2.2 Explore the GUI

Click on the triangle to the left of *suite conf* to expand that section. Click on *Build and run switches*. A panel will appear on the right-hand side containing options for controlling what tasks will be run for this suite. You can see that it will build the UM and reconfiguration executables, run the reconfiguration and then run the model.

Note: We generally use a **common notation** to help users navigate through the GUI and to help us help you with questions. Getting to "UM Science Settings" would be indicated like this: $um \rightarrow namelist \rightarrow UM$ *Science Settings*. This notation will be used throughout the rest of this tutorial.

The input namelists for the UM are contained in the *um* -> *namelist* section. Let's take a look at the science namelist for *Microphysics (Large Scale Precipitation)*, run_precip under *UM Science Settings*.

For each UM namelist item there is a short description to help you understand what that variable is. Click on the cog next to a namelist variable and select *Help* to view more detailed information. The help information can give you some useful pointers but be aware that it has been written with Met Office setup in mind.

Range and type checking of variables is done as soon as the user enters a new value. Try changing the value of timestep_mp_in to 0. This will cause an error flag to appear, hover over the error for more information and click the *undo* button several times to revert to the original value.

Some larger science sections have been been divided into subsections; take a look at *Section 05 - Convection* for an example of this. To open a section in a new tab click with the middle mouse button, expand the section by clicking the page triangles. Rose edit has a search box which can be used to search item names. Try searching for the variable astart where the input dump is specified, you will be taken directly to the *Dumping and Meaning* panel.

Trigger ignored settings are hidden by default and only appear to the user when the appropriate options are selected. Open the *Gravity Wave Drag* panel, if you change <code>i_gwd_vn</code> from 5 to 4 the options available change. Click the *save* button to apply these changes to your app. Let's take a look at what effect this has had to the <code>rose-app.conf</code> file, run <code>fcm diff</code> in the suite directory.

```
puma2$ cd \sim/roses/u-ag137 puma2$ fcm diff -g
```

You should see that several namelist items have had !! added to the start of the line. This tells Rose to ignore these items when processing the app file into Fortran namelists. Should you wish to see all variables on a panel select *View All Ignored Variables* and *View Latent Variables* from the *View* menu.

Switch back to the Rose edit window and click the *Undo* button to revert the changes and then *Save* the suite again. To view all changes made to the suite in the current session go to *Edit > Undo/Redo Viewer*.

2.2.3 Error checking of UM inputs

In addition to the type and range checking of namelist items and environment variables, more thorough checks can be made using Rose macros and the fail-if/warn-if metadata.

First let's check if the suite contains any options which trigger the fail-if and warn-if checks in the UM metadata. Select menu item *Metadata > Check fail-if*, *warn-if*. As this suite is setup correctly FailureRuleChecker: No problems found should appear at the bottom right of the window.

Now let's try and introduce both a warning and a failure. We're going to change the boundary layer option alpha_cd. Either navigate to Section 03 - Boundary Layer -> Implicit solver options or type alpha_cd into the search bar. Click on the + sign to add an array element to alpha_cd and type 1.5 into the new box. Next navigate to Reconfiguration and Ancillary Control -> Output dump grid sizes and levels and increase the number of ozone levels to 86. Now run the fail-if, warn-if checker again.

- What is the error?
- What is the warning?

Use the *Undo* button to put the settings back to how we found them and run the checker again. It is strongly recommended that whenever namelists and environment variables are modified that the fail-if, warnif checker is applied before running the suite.

RUNNING A UM SUITE ON ARCHER2

3.1 ARCHER2 architecture

In common with many HPC systems, ARCHER2 consists of different types of processor nodes:

- Login nodes: This is where you land when you ssh into ARCHER2. Typically these processors are used for file management tasks.
- **Compute / batch nodes:** These make up most of the ARCHER2 system, and this is where the model runs.
- **Serial / post-processing nodes:** This is where less intensive tasks such as compilation and archiving take place.

ARCHER2 has two file systems:

- /home: This is relatively small and is only backed up for disaster recovery.
- /work: This is much larger, but is not backed up. Note that the batch nodes can only see the work file system. It is optimised for parallel I/O and large files.

Consult the ARCHER2 website for more information: http://www.archer2.ac.uk

3.2 Running a Standard Suite

To demonstrate how to run the UM through Rose we will start by running a standard N48 suite at UM13.0.

3.2.1 Copy the suite

- In rosie go locate the suite with idx **u-cc519** owned by **rosalynhatcher**.
- Right click on the suite and select *Copy Suite*.

This copies an existing suite to a new suite id. The new suite will be owned by you. During the copy process a wizard will launch for you to edit the suite discovery information, if you wish.

A new suite will be created in the MOSRS rosie-u suite repository and will be checked out into your ~/ roses directory.

3.2.2 Edit the suite

• Open your new suite in the Rose config editor GUI.

Before you can run the suite you need to change the userid, queue, account code and reservation:

- Click on *suite conf* -> *jinja2* in the left hand panel
- Set HPC_USER (that's your ARCHER2 username)

If following the tutorial as part of an organised training event:

- Set HPC_ACCOUNT to 'n02-training'
- Set HPC_QUEUE to 'standard'
- Ensure RESERVATION is set to **True**
- Set HPC_RESERVATION to be the reservation code for today. (e.g. 'n02-training_1055426')

If following the tutorial as self-study:

- Set HPC_ACCOUNT to the budget code for your project. (e.g. 'n02-cms')
- Set HPC_QUEUE to 'short'
- Set RESERVATION to False

Notes

- Quotes around the variable values are essential otherwise the suite will not run.
- In normal practice you submit your suites to the parallel queue (either **short** or **standard**) on ARCHER2.
- For organised training events, we use processor reservations, whereby we have exclusive access to a prearranged amount of ARCHER2 resource. Reservations are specified by adding an additional setting called the reservation code; e.g. **n02-training_226**.
- Save the suite (*File > Save* or click the *down arrow* icon)

3.2.3 Run the suite

The standard suite will build, reconfigure and run the UM.

• Click on the triangle symbol on the right end of the menu bar to run the suite.

Doing this will execute the rose suite-run command (more on this later) and start the Cylc GUI through which you can monitor the progress of your suite graphically. The Cylc GUI will update as the job progresses.

3.2.4 Looking at the queues on ARCHER2

While you're waiting for the suite to run, let's log into ARCHER2 and learn how to look at the queues.

Run the following command:

```
squeue -u <archer2-user-name>
```

This will show the status of jobs you are running. You will see output similar to the following:

```
ARCHER2> squeue -u ros

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

148599 standard u-cc519. ros R 0:11 1 nid001001
```

At this stage you will probably only have a job running or waiting to run in the serial queue. Running squeue will show all jobs currently on ARCHER2, most of which will be in the parallel queues.

Once your suite has finished running the Cylc GUI will go blank and you should get a message in the bottom left hand corner saying Stopped with succeeded.

Tip: Cylc is set up so that it *polls* ARCHER2 to check the status of the task, every 5 minutes. This means that there could be a maximum of 5 minutes delay between the task finishing on ARCHER2 and the Cylc GUI being updated. If you see that the task has finished running but Cylc hasn't updated then you can manually poll the task by right-clicking on it and selecting *Poll* from the pop-up menu.

3.3 Standard Suite Output

The output from a standard suite goes to a variety of places, depending on the type of the file. On ARCHER2 you will find all the output from your run under the directory ~/cylc-run/<suitename>, where <suitename> is the name of the suite. This is actually a symbolic link to the equivalent location in your /work directory (E.g. /work/n02/n02/<username>/cylc-run/<suitename>.

3.3.1 Task output

Note: Rose Bush is a web-based tool for viewing the standard output and errors from suites. Unfortunately this does not work on the current puma server, so we need to browse the log files directly.

Note: To run Rose Bush on Monsoon run: firefox http://localhost/rose-bush

On PUMA2, navigate to the cylc-run directory:

```
cd ~/cylc-run/<suitename>
ls
```

You should see directories for each of the suites that you have run. Go to the suite you have just run and into the log directory:

```
cd <suitename>/log/job/1
ls
```

You will see directories for each of the tasks in the suite. For this suite there are 4 tasks: fcm_make (code extraction), fcm_make2 (compilation), recon & atmos. Try looking in one of the task directories:

```
cd recon/NN
ls
```

Here NN is a symbolic link created by Rose pointing to the output of the most recently run. You will see several files in this directory. The job.out and job.err files are the first places you should look for information when tasks fail.

3.3.2 Compilation output

The output from the compilation is stored on the host upon which the compilation was performed. The output from fcm_make is inside the directory containing the build, which is inside the share subdirectory.

```
~/cylc-run/<suitename>/share/fcm_make/fcm-make2.log
```

If you come across the word "failed", chances are your model didn't build correctly and this file is where you'd search for reasons why.

3.3.3 UM standard output

The output from the UM scripts and the output from PEO of the model are written to the job.out and job.err files for that task. Take a look at the job.out for the atmos task, by opening the following file:

```
~/cylc-run/<suitename>/log/job/1/atmos/NN/job.out
```

• Did the linear solver for the Helmholtz problem converge in the final timestep?

Job Accounting

The sacct command displays accounting data for all jobs that are run on ARCHER2. sacct can be used to find out about the resources used by a job. For example; Nodes used, Length of time the job ran for, etc. This information is useful for working out how much resource your runs are using. You should have some idea of the resource requirements for your runs and how that relates to the annual CU budget for your project. Information on resource requirements is also needed when applying for time on the HPC.

Let's take a look at the resources used by your copy of u-cc519 run.

• Locate the SLURM Job Id for your run. This is a 6 digit number and can be found in the job. status file in the cylc task log directory. Look for the line CYLC_BATCH_SYS_JOB_ID= and take note of the number after the = sign.

Run the following command:

```
sacct --job=<slurm-job-id> --format="JobID, JobName, Elapsed, Timelimit, NNodes"
```

Where <slurm-job-id> is the number you just noted above. You should get output similar to the following:

ARCHER2-ex> sacct --job=204175 --format="JobID, JobName, Elapsed, Timelimit, →NNodes"

Ċ	JobID	JobName	Elapsed	Timelimit	NNodes
204175		u-cc519.a+	00:00:23	00:20:00	1
204175.k	oatch	batch	00:00:23		1
204175.6	exte+	extern	00:00:23		1
204175.0	0	um-atmos.+	00:00:14		1

The important line is the first line.

- How much walltime did the run consume?
- How much time did you request for the task?
- How many CUs (Accounting Units) did the job cost?

Hint: 1 node hour currently = 1 CU. See the ARCHER2 website for information about the CU.

There are many other fields that can be output for a job. For more information see the Man page (man sacct). You can see a list of all the fields that can be specified in the --format option by running sacct --helpformat.

3.3.4 Binary output - work and share

By default the UM will write all output to the directory it was launched from, which will be the task's work directory. However, all output paths can be configured in the GUI and in practice most UM tasks will send output to one or both of the suite's work or share directories.

```
~/cylc-run/<suitename>/work/1/atmos
or
~/cylc-run/<suitename>/share/data
```

For this suite output is sent to the work directory.

Change directory to the work space.

• What files and directories are present?

Model diagnostic output files will appear here, along with a directory called pe_output. This contains one file for each processor, for both model and reconfiguration, which contain logging information on how the model behaved.

Open one of these files <suite-id>.fort6.peXX in your favourite editor.

The amount of output created by the suite and written to this file can be controlled in the suite configuration $(um \rightarrow env \rightarrow Runtime\ Controls \rightarrow Atmosphere\ only)$. For development work, and to gain familiarity with the system, make sure "Extra diagnostic messages" are output. Switch it on in this suite if it isn't already.

It is well worth taking a little time to look through this file and to recognise some of the key phrases output by the model. You will soon learn what to search for to tell you if the model ran successfully or not. Unfortunately, important information can be dotted about in the file, so just examining the first or last few lines may not be sufficient to find out why the model hasn't behaved as you expected. Try to find answers to the following:

- How many prognostic fields were read from the start file?
- How many boundary layer levels did you run with?
- What was the range of gridpoints handled by this processor?

Check the file sizes of the different file types. The output directory will contain start dumps, diagnostic output files and possibly a core dump file if the model failed and these usually have very different sizes.

SECTION

FOUR

FCM TUTORIAL

In this section you will learn about:

- Incorporating modifications to your suite
- Creating a ticket to document your code change
- Creating a branch using the FCM GUI and command line
- How to checkout and change a working copy
- Getting information about your working copy and branch
- Committing changes to your branch
- · Version control of suites

4.1 Setting up your default text editor

When you attempt to create a branch or commit changes to the repository, you will normally be prompted to edit your commit log message using a text editor. The system chooses its editor by searching for a non-empty string through a hierarchy of environment variables in this order: SVN_EDITOR, VISUAL, and EDITOR.

The editor you select must able to run in the foreground. The default editor is vi. If you prefer to use emacs or nedit, for example, you can add one of the following in your \$HOME/.profile, \$HOME/.kshrc (Korn) or \$HOME/.bashrc (Bash):

```
# Emacs
export SVN_EDITOR=emacs
# NEdit
export SVN_EDITOR='nedit'
```

4.2 Applying modifications to a UM suite

Now that you've run a basic suite, you need to know how to apply changes to the trunk code. We'll start by applying existing changes (aka a branch) to your suite. A branch equates to a copy of the UM source code tree with user modifications. A branch can contain changes to many code files.

As a user, you will be supplied with the **URL** and possibly a version number of a branch. FCM keywords can be used to specify the URL which is a way of using shorthand for standard bits of the URL path. For example, this branch has been created in the MOSRS UM repository:

A shorter way to specify this is:

fcm:um.x-br/dev/rosalynhatcher/vn13.0_training_um_shell1

This branch contains a code change to um_shell to print:

Tutorial Change: Start of UM RUN Job: instead of Start of UM RUN job:

To add this branch go to the panel fcm_make -> env -> sources and click the + button next to um_sources to add a new branch URL:

branches/dev/rosalynhatcher/vn13.0_training_um_shell1

Now *Save* your suite and then submit it either by running rose suite-run or clicking the "Play" button in the rose edit GUI.

When the suite has completed, check the job.out file to verify that you have got the changed output message:

Tutorial Change: Start of UM RUN Job: instead of Start of UM RUN job:

4.3 Opening a Ticket

All code changes destined for the UM trunk must have an associated Trac Ticket documenting the change (e.g. https://code.metoffice.gov.uk/trac/um/ticket/1957). For all other changes creating a ticket to document your change is entirely optional.

Note: For full details on the UM working practices including the review and commit to trunk process please see https://code.metoffice.gov.uk/trac/um/wiki/working_practices. If you are planning to make a code change intended for the trunk please make sure you read this before starting the change.

We will now create a ticket for our code change. Navigate to the UM Trac page on MOSRS: https://code.metoffice.gov.uk/trac/um (You will be prompted to login to MOSRS if you haven't already done so). Click on *New Ticket*. A form entitled **Create New Ticket** should appear. For the purposes of this tutorial fill in the following:

- Summary: "Code change for UM Tutorial"
- **Description**: provide as much detail as possible so that all reading the ticket are able to understand the planned change. You can use WikiFormatting to enhance the readability of your text.
- Type: select "task"
- **Milestone**: select "*Not for Builds*"; this indicates the ticket is not intended for the UM trunk. If your change is intended for the trunk this should be set to the UM release the change is being targeted at: e.g. "*UM13.0 code release*"
- Severity: leave this as "minor"
- Component: select "General"
- cc: leave this empty

• Owner: assign the ticket to yourself by selecting your username from the drop down list.

A preview of your ticket should appear at the bottom of the page. If if doesn't appear automatically, use the *Preview* button to inspect your ticket before clicking *Create ticket* button to create the ticket.

Remember the number of your new ticket as you will need it later in this tutorial.

4.4 Making Code Changes

The default text editor for entering commit messages is vi. If you would prefer to use a different editor; for example emacs or vim, please see the section on "Setting up your default text editor".

4.4.1 Creating a branch

Firstly create a new directory (e.g. um/branches) in your \$HOME directory on PUMA2 which will be your work area and cd to it.

Create a new branch by running the command:

```
fcm branch-create -k <ticket> <branch_name> fcm:um.x-tr@vn13.0
```

Where:

- <ticket> is the related Trac ticket number for the ticket you created earlier.

You will be prompted to edit the message log file. A standard template is automatically supplied and pops up in your default text editor. Add a comment about what the branch is for at the top of the file. When you are ready, save your change and exit the editor. Answer y when you are prompted to go ahead and create the branch.

If the branch is created successfully you will get a message similar to the following:

The branch will have a URL (location in repository) like this:

```
https://code.metoffice.gov.uk/um/main/branches/dev/[userid]/vn13.
0_[branch_name]
```

By default FCM prepends the revision of the trunk you have branched from to your branch name. Here, as we have used version labelling it is vn13.0. If you had entered a version number instead of a label FCM would have added rxxx where xxx is the revision number instead.

Note: For further information on the options available for branch creation type: fcm branch-create --help

Take a note of the revision number the branch was created at, and the branch name, vn13. 0_[branch_name].

You can see your branch from within the MOSRS Trac (https://code.metoffice.gov.uk/trac/um): Click on *Browse Source* on the Trac menu bar and then navigate through *main* -> *branches* -> *dev*-> [userid]

Your branch will also appear in the UM repository mirror held on PUMA2 (within 5 minutes)

4.4.2 Making changes to a working copy

Checking out a working copy

You may have noticed that creating a branch does not create a source code tree that you can edit (working copy)! To do this you need to checkout your branch. Make sure you have changed to the working directory you created earlier as by default code is checked out to the current directory. To checkout a copy of the UM code type:

```
fcm checkout URL
```

Where URL is the url of your branch. This can be supplied in its full form:

```
https://code.metoffice.gov.uk/svn/um/main/branches/dev/[userid]/vn13.
0_[branch_name]
```

or by a shorter way:

```
fcm:um.x-br/dev/[userid]/vn13.0_[branch_name]
```

Note:

- In the second form we have replaced the leading part of the Subversion URL https://code.metoffice.gov.uk/um/main/branches with the FCM repository keyword fcm:um.x-br. Keywords are shortcuts to save you from having to type in the full URL.
- As we have not specified a local directory PATH in the checkout command, it will create a working copy in your current working directory, using the basename of the URL you are checking out. For example, when you checkout the branch you have just created, the command should create the working copy in \$PWD/vn13.0_[branch_name]. Make a note of the location of your working copy, in case you forget where you have put it.
- We are also not specifying a revision to checkout, so it will checkout the HEAD, i.e. the latest revision.

Changing code

Back in the work area directory you created at the beginning of branch creation you should now see that a new directory has appeared and that it is named the same as your branch. This is your *working copy*. cd into this directory and explore the code structure to familiarise yourself with how the code is structured.

Now make some code changes! Use the following scenario to take you through the basic method of changing, adding and deleting files:

- Change to the src/control/top_level/ sub-directory in your working copy.
- Edit um shell.F90, using your favourite editor
- Go to the line that says CALL umPrint('I am PE '//TRIM(str(mype))//' on '//TRIM(env_myhost),
- Change: 'I am PE' to 'Hello World PE'

- Go to the line that says of UM RUN Job:
- Change: of UM RUN Job : to of UM Tutorial RUN Job:
- Save your changes and Exit the editor

Adding a new file

• Still in the src/control/top_level directory, add a new FORTRAN module file um_training_mod.F90 containing a subroutine called um_training_sub().

Hint:

- An example file is available on PUMA2: ~um1/um-training/um_training_mod.F90.
- The routine umPrint should be used for writing out messages rather than standard FORTRAN WRITE statements.
- Run fcm add on the command line, to let the repository know you're adding a new file at the next commit. Make sure you are still in src/control/top_level and then type:

```
fcm add um_training_mod.F90
```

at the command prompt.

• Modify um_shell.F90 to use this new module. You'll see lots of USE statements near the top of the file. Add the following to use our new one.

```
USE um_training_mod
```

• Then add a line to call the um_training_sub subroutine (suggest around line 903 within the um_Shell_banner subroutine):

```
CALL um_training_sub()
```

Deleting a file

- In the fcm-make/ncas-xc30-ifort directory, you should see a file um-createbc-safe. cfg
- Run fcm delete on the command line, to let the repository know you want to remove this file from your branch: Make sure you are in fcm-make/ncas-xc30-ifort and then type:

```
fcm delete um-createbc-safe.cfg
```

Getting information about changes to a working copy

All the changes you have made so far have not been committed - i.e. saved to your branch in the repository. It is possible to list these changes using the fcm status command. Firstly, make sure you cd back up to the top level of your working directory and then type:

```
fcm status
```

and you should see a list of files that have been changed. If you've followed the example scenario above you should see output similar to this:

```
ros@puma2$ fcm status
D          fcm-make/ncas-xc30-ifort/um-createbc-safe.cfg
M          src/control/top_level/um_shell.F90
A          src/control/top_level/um_training_mod.F90
```

Notice that each changed file is flagged with a letter that indicates what the change was: A for Added, D for Deleted and M for Modified.

Reverting an uncommitted change

At this point you can undo any changes before committing. Try the following so that you know how to restore a changed file:

- Edit src/control/top_level/initial_4A.F90 to make any change and then save it.
- Run fcm status again to confirm it has been flagged as Modified.
- Run fcm revert on the command line: Make sure you are still in src/control/top_level and then type fcm revert initial_4A.F90
- Re-run fcm status to see that the file is no longer modified.

Note that fcm revert will undo ALL changes to a file relative to your branch. Therefore if you've made several uncommitted changes, fcm revert will undo them all, not just the last one.

4.4.3 Committing changes

The change in your working copy remains local until you commit it to the repository where it becomes permanent. If you are planning to make a large number of changes, you are encouraged to commit regularly to your branch at appropriate intervals. Make sure you are in the top level directory of the working copy and then type:

```
puma2$ fcm commit
```

A text editor will appear to allow you to edit the commit message. You must add a commit message to describe your change above the line that says ——Add your commit message ABOVE — do not alter this line or those below——. Your commit will fail if you do not enter a commit message. Make sure you provide meaningful commit messages (if your change is intended for inclusion in the trunk you should reference your ticket number) as these will show up in the revision logs and can be a useful source of information.

Tip: DO:

- Put a link to the ticket that raises the issues you are addressing using a wiki syntax; e.g. #15. Putting this as the first item in the commit message means it will show very clearly under Trac what ticket the change relates to.
- State the reason for the change
- List possible impacts to other users
- Use wiki syntax that can be displayed nicely in plain text

DON'T:

• Repeat what's already stated in the merge template; e.g. statements such as merge my branch to the trunk should be avoided

- List the files you have changed. This will already have been included in the commit log by FCM
- Use wiki syntax that cannot be displayed nicely in plain text
- Be vague. A commit message that just says Fix is insufficient!

Save your change and exit the editor. Answer y when you are prompted to confirm the commit.

If you've followed the example scenario above you should see output similar to this:

```
ros@puma2$ fcm commit
[info] vi: starting commit message editor...
Change summary:
              _____
[Root : https://code.metoffice.gov.uk/svn/um]
[Project: main]
[Branch: branches/dev/rosalynhatcher/vn13.0_tutorial]
[Sub-dir: ]
      fcm-make/ncas-xc30-ifort/um-createbc-safe.cfg
      src/control/top_level/um_shell.F90
M
      src/control/top_level/um_training_mod.F90
Commit message is as follows:
______
#7107 Testing FCM Tutorial
______
Would you like to commit this change?
Enter "y" or "n" (or just press <return> for "n"): y
Deleting fcm-make/ncas-xc30-ifort/um-createbc-safe.cfg
Sending
           src/control/top_level/um_shell.F90
           src/control/top_level/um_training_mod.F90
Adding
Transmitting file data ..done
Committing transaction...
Committed revision 113821.
Updating '.':
At revision 113821.
```

4.4.4 Getting information about your branch

If you need to find out information about your (or another user's) branches, you can use the fcm branch info command.

In the directory where you checked out the code, type:

```
puma2$ fcm branch-info
```

You should see information about your branch revision, when it was last changed and the parent it was created from:

```
ros@puma2$ fcm branch-info
URL: https://code.metoffice.gov.uk/svn/um/main/branches/dev/rosalynhatcher/
→vn13.0_tutorial
Repository Root: https://code.metoffice.gov.uk/svn/um
Revision: 113821

(continues on next page)
```

(continued from previous page)

```
Last Changed Rev: 113821

Last Changed Date: 2022-11-18T10:44:16.243200Z

Branch Create Author: rosalynhatcher

Branch Create Rev: 113820

Branch Create Date: 2022-11-18 10:33:08 +0000 (Fri, 18 Nov 2022)

Branch Parent: https://code.metoffice.gov.uk/svn/um/main/trunk@111272

Merges Avail From Parent: 113812 113786 ..... 111763 111761 111757 111726

Merges Avail Into Parent: 113821
```

4.4.5 Testing that your branch works

Now that you have made a branch you can use it in the suite you were running earlier. Go back to the section where you added an existing branch to your suite and add your new branch as well.

Save and then Run your suite.

If you have followed the tutorial scenario so far you should find that your suite fails during the fcm extract of code. In the job.err file for the fcm_make task you will see an error message like this:

```
[FAIL] um/src/control/top_level/um_shell.F90: merge results in conflict
           merge output: /home/ros/cylc-run/u-cc519-test/share/fcm_make/
[FAIL]
.fcm-make/extract/merge/um/src/control/top_level/um_shell.F90.diff
           source from location 0: svn://puma2.archer2.ac.uk/um.xm svn/main/
→trunk/src/
control/top_level/um_shell.F90@111272
           source from location 1: svn://puma2.archer2.ac.uk/um.xm_svn/main/
[FAIL]
→branches/
dev/rosalynhatcher/vn13.0_training_um_shell1/src/control/top_level/
um_shell.F90@113821
[FAIL] !!! source from location 2: svn://puma2.archer2.ac.uk/um.xm_svn/main/
⇒branches/
dev/rosalynhatcher/vn13.0_tutorial/src/control/top_level/
um shell.F90@113821
```

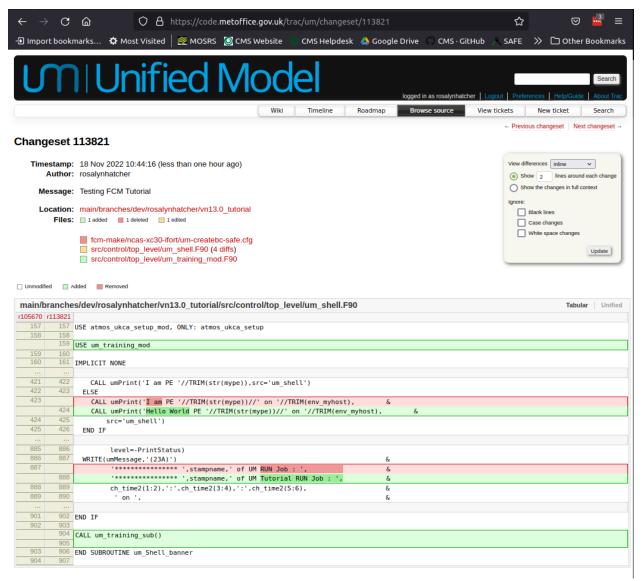
This is because the sample branch and your branch contain modifications to the same line in file um_shell. F90 and so conflict. Errors like this can be quite common if you are working with others on the same section of code. The default behaviour of FCM in this situation is to fail and force you to resolve the conflict. For the purposes of this exercise we will simply remove the um_shell1 branch from the suite and rerun it - we've decided we only want the changes we've put in our branch. In practice you will need to go through the process of resolving a conflict which can be quite complex. There is a tutorial dedicated to conflict resolution should you wish to know more and is a good reference should you encounter conflicts in your development work.

• Check that you can see the changed print statements and that the subroutine um_training_sub was called.

Hint: Remember not all run output is in the job.out or job.err files. You may need to look in the pe_output directory too.

4.4.6 Viewing your changes in Trac

Making a change to your branch results in a **changeset** which is basically a record of the changes. One way of viewing the changeset you have just created is to click on *Timeline* in Trac. The Timeline view is a sequential record of all events in the repository. Near the top, you should see changesets for the creation of your branch, and the subsequent commit for the code changes you made. The changesets are numbered corresponding to the revision of your branch which would have been displayed in the GUI when you did a fcm commit or `fcm branch info. To see all the details click on the line '*Changeset[xxx]*...' relating to your changeset. Alternatively, if you enter the number of the changeset "[xxx]" into the search box at the top right, it will take you directly to the numbered changeset. Your changeset should look something like this:



4.5 Documenting your change

Go back to the Trac ticket you created for your code change and add some documentation as follows:

- Add a link to your branch:

 Development branch: [source:main/branches/dev/<username>/<branch_name>]
- A description of what code has changed
- Test results (i.e. Did your suite run? Were there any clashes to resolve?)
- Any other information you want to add
- As we have finished the change for this tutorial example we will resolve the ticket as **fixed** by clicking *Modify Ticket* `and selecting *resolve & assign to <username> as fixed*.

Preview and Submit your ticket to save the changes. Check the link you added works.

4.6 Tidying Up

If your development is destined for the UM trunk, then once you have finished your code changes and it has been tested and reviewed, your branch will be committed to the project shared package branch by the project owner. Once this has been done and there are no problems, your branch is essentially redundant. If no other users are using this branch in their suites it can be deleted.

For the purposes of this tutorial, you can now proceed to delete your branch. When you delete a branch, it becomes invisible from the HEAD revision, but will continue to exist in the repository should you want to refer to it in the future.

List branches owned by you

If you forget what your branch is called and/or what other branches you have created, you can get a listing of all the branches you have created in a project. To do this use the following command:

```
fcm branch-list URL
```

Where URL is the name of repository you want to search. In this case it would be fcm:um.x

Delete a branch

Make sure you are in the relevant working copy directory and type:

```
fcm branch-delete
```

You will be prompted to edit the commit message file. Again a standard template is automatically supplied for the commit. Add your commit message, save your changes and exit the editor.

Answer y when you are prompted to go ahead and delete this branch.

Your working copy is now pointing to a branch that no longer exists at the HEAD revision of the repository. It is possible to keep this working copy, create a new branch and switch your working copy to point to the new branch. Otherwise, you can remove your working copy by issuing a careful rm -rf command.

4.7 Version Control of Suites

Just like the model code, your UM suites are also under version control in a subversion repository called roses-u which is on the MOSRS. Once you have a working copy of your suite under ~/roses you can use FCM commands in the same way as for your source code branches; i.e. commit changes, diff changes, etc.

• Look in the roses-u repository via MOSRS Trac (https://code.metoffice.gov.uk/trac/roses-u) and find the suite you created in the previous section.

Hint: Go to *Browse Source* 'then drill down to find your suite. e.g. u-cc519 would be under c/c/5/1/9

- When was the suite last modified?
- Go to your suite working directory and type fcm status to see the changes you have made since you copied the suite.
- Run fcm commit to commit your changes to the repository.
- Look again in the MOSRS roses-u Trac and see that your commit has now appeared in the repository. What is the suite's last modified time now?
- Use Trac to view the changes you have made to the suite.

Hint: Click on the number in the revision column, and then on the *View changes* button to show a diff of your changes

SOLVING COMMON UM PROBLEMS

This section exposes you to more typical UM errors and hints at how to find and fix those errors.

You may encounter other errors, often as a result of mistyping, for which solution hints are not provided.

5.1 Set up N96 GA7.0 AMIP example suite

Find and make a copy of suite u-cc654.

Firstly make the essential changes required to run the suite. That is:

- The account code ('n02-training' if you're on an organised training event)
- Your ARCHER2 user name
- The queue to run in.

Hint: Look in the *suite conf* section. For organised training events you will see that this suite is setup to use reservations listed as Tuesday, Wednesday, Thursday; select the appropriate day. For self-study switch off "Use a reservation on ARCHER2" and select the short queue.

• Did you manage to find where to set your ARCHER2 username?

This suite is set up slightly differently to the one used in the previous sections; suites do vary on how they are set up but you will soon learn where to look for things. This suite is set up so that specifying your username on the remote HPC is optional.

- Click View -> View Latent Variables. You should see Username on ARCHER2 appear in the panel greyed out.
- Click the + sign next to it and select *Add to configuration*
- Enter your ARCHER2 username

5.2 Errors resolved in the code extraction

Save the suite and then Run it either from the GUI or the command line.

The suite should fail in the fcm_make_um task. This is the task that extracts all the required code from the repository including any branches. The failure will be indicated in the Cylc GUI with a red square and the state failed.

• What is the error?

Hint: Examine the job.err and job.out to find the cause of the problem. You can view these files quickly and easily directly from the Cylc GUI. **Right-click** on the failed fcm_make_um task and select *View -> job stderr*

This indicates that the branch cannot be found due to an incorrect branch name. You will need to look at the UM code repository through Trac on MOSRS (https://code.metoffice.gov.uk/trac/um/browser) to determine the correct name.

Fix the error, Save the suite.

Now we will stop the suite and then re-run it. In the Cylc GUI click on *Control* > *Stop Suite* and then select *Stop now* and then click on *OK*. *Run* the suite again.

The suite will fail in the fcm_make_um task again.

• What is the error?

Hint: Again look in the job.err file. This kind of error results when changes made in two or more branches affect the same bit of code and which the FCM system cannot understand how to resolve.

• Which file does the problem occur in?

In practice, you will need to fix the problem with the code conflict as you did in the FCM tutorial section. To proceed in this case, navigate to <code>fcm_make_um</code> -> <code>sources</code> and remove the branch called <code>vn11.7_training_merge_error</code> by clicking on it and then clicking the - sign.

Save the suite.

Last time we stopped the suite and then re-ran it, however, it is possible to reload the suite definition and then re-trigger the failed task without first stopping the running suite. To do this change to the suite directory:

```
puma2$ cd ~/roses/<suitename>
```

We then reload the suite definition by running the following Rose command:

```
puma2$ rose suite-run --reload
```

Wait for this command to complete before continuing. Finally in the Cylc GUI *right-click* on the failed task and select *Trigger* (*run now*). The fcm_make_um task will then submit again.

• Is there an error in fcm_make_um this time?

If you look in the job.err file now it should be empty and the job.out file indicates SUCCESS.

5.3 Errors resolved in the compile and run

- Has the fcm_make2_um (compilation) task completed successfully?
- You should have a failure. Open the job.err file what does it indicate?
- Which routine has an error?
- What is the error?
- What line of the Fortran file does it occur on?

In practice, you would need to fix the error in your branch on PUMA2 and then restart the suite. In this case, navigate to *fcm_make_um -> sources* and remove the branch vn11.7_training_compile_error. *Save* the suite, *Shutdown* or *Stop* the failed run and then *Run* it again.

Tip: This time we chose to shutdown the failed suite rather than do a reload. In this scenario we need to redo the code extraction (fcm_make_um) step so doing a reload would be slightly more complex; you would need to *Reload* and then *Re-trigger* both the fcm_make_um and the fcm_make2_um tasks. With experience you get to know when it's better to do a *Reload* and when to *Shutdown* a suite.

Note again that the task submitted successfully.

- Did the fcm_make2_um task succeed this time?
- What about the install_cold task?
- What is the error?
- Does the start dump exist?
- What is the name of the correct start dump?

Hint: Look in the directory where it thinks the start file should be - is there a candidate in there?

Point your suite to the correct start dump. Fixing this problem isn't quite as easy as it sounds. A search in the Rose edit GUI for the dump file name ab642a.da19880901_00_err will not locate anything. For this suite it is not possible to fix this issue through the GUI, for some other suites you can edit the initial dump location in the panel $um \rightarrow namelist \rightarrow Reconfiguration$ and Ancillary Control \rightarrow General technical options.

Suites can be and are set up differently and there will be times when you need to edit the cylc suite definition files directly.

In your suite directory on PUMA2 (~/roses/<suitename>) use grep -R to search for the start dump name ab642a.da19880901_00_err in the suite files. You should see 2 occurrences listed

Edit the dump name in the appropriate .rc file for the HPC we are running on, to point to the correct initial dump file.

Hint: This suite is set up to run on multiple platforms, make sure you edit the file appropriate to ARCHER2. You may notice that AINITIAL is set 3 times; a different file is required depending on the resolution the model is being run at. This suite is running at N96 resolution.

Reload the suite definition and then *Re-trigger* the install_cold task. The task should succeed this time.

• Has the model run successfully?

This time the model should have failed with an error.

• What is the error message?

Hint: Try searching for ERROR - you will soon learn common phrases to help track down problems.

Note: If you use the search job.err box at the bottom of the gcylc viewer, when you select *Find Next* you will see a message indicating the live feed will be disconnected. Click *Close*.

• Which PE Ranks signalled the Abort?

In general it can be useful to note which processors failed and then look at the detailed output for those processors. In this scenario, however, all the processors aborted. We'll now take a look at the individual PE output file. Change to the pe_output directory for the atmos_main task. This is under ~/cylc-run/<suite-id>/work/<cycle>/atmos_main/pe_output.

Open the file called <suite-id>.fort6.pe0. Sometimes extra information about the error can be found in the individual PE output files.

• At what timestep did the error occur?

The error message indicates that the model has suffered a convergence failure in the routine EG_BICGSTAB_MIXED_PREC. This basically means that the model was not able to find a solution to the requested accuracy with the amount of effort specified. In this case the failure results from the value chosen for gcr_max_iterations. You could try to find what setting similar models use (with the MOSRS repository you have access to all model setups) or looking at the help within rose edit may point you in the right direction. Go to $um \rightarrow namelist \rightarrow UM$ Science Settings \rightarrow Sections 10 11 12 - Dynamics settings \rightarrow Solver and set it to the suggested value. Save, Reload and Re-trigger.

The model should fail with the same error. So what's gone wrong here? We've changed the value of the number of iterations to a recommended value so why didn't it work? The first thing to check is that the new value has indeed been passed to the model. We do this by checking the variable in the namelists which are written by the Rose system. On ARCHER2 navigate to the work directory for the atmos_main task (ie. ~/cylc-run/<suite-id>/work/<cycle>/atmos_main). In here you will see several files with uppercase names (e.g. ATMOSCNTL, SHARED), these contain the Fortran namelists which are read into the model. Have a look inside one of them to see the structure. Now search (use *grep*) in these files for the max number of solver iterations variable gcr_max_iterations.

Hint: Search for the string gcr_max_iterations=.

• What value does it have? Is this what you changed it to in the Rose edit GUI?

So why was the change not picked up? Go back to view the setting in the Rose GUI. By the side of the variable gcr_max_iterations there is a little icon of a hand on paper, this indicates that there is an "optional configuration override" for this variable.

Optional configuration overrides add to or overwrite the default configuration. They are useful to make it easier to switch between different configurations of the model. For example switching between different resolutions.

Click on the icon and the list of overrides appears. You will see that the variable is set to 1 in the *training* override file and it is this value that is being used in the model. Unfortunately optional configuration override files cannot be changed through the GUI so we will need to edit the Rose file directly. Override files for the um app live in the directory ~/roses/<suite-id>/app/um/opt. Open the file rose-app-training.conf and edit the value for gcr_max_iterations. *Save*, *Reload* and *Retrigger* the suite.

Check the gcr_max_iterations variable in the namelist file again to confirm that it does now have the correct value. This time the model should run successfully. Check the output to confirm that there are no errors. Check that the model converged at all time steps.

FURTHER EXERCISES (1)

Now that we have built the suite, there is no need to rebuild it each time you run it. Switch off compilation of the UM and reconfiguration.

Hint: See the *suite conf* section in the Rose edit GUI.

6.1 Change the model output logging behaviour

Navigate to um -> namelist -> Top Level Model Control -> Run Control and Time Settings.

Set ltimer to True. Timer diagnostics outputs timing information and can be very useful in diagnosing performance problems.

Save and Run the suite.

Check the output from processor 0 in the `fort6.pe000` file.

- Which routine took the most time?
- How many times was Atm_Step called?
- How many time steps did the model run for?
- Which PE was the slowest to run AP2 Boundary Layer? Which was the fastest?

Switch on "IO timing"

Hint: Look in the *IO System Settings* panel.

Re-run the model and search for "Total IO Timings" in the job.out file.

6.2 Change the processor decomposition

Navigate to *suite conf* -> *Domain Decomposition* -> *Atmosphere*.

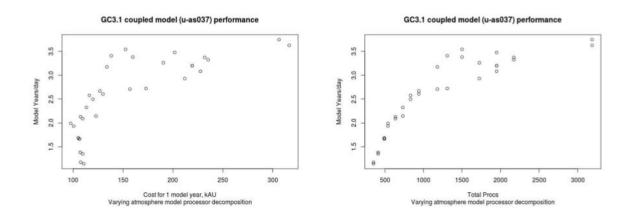
- What is the current processor decomposition?
- Why is this not a good way to run the model?

Hint: The base ARCHER2 charging unit is a node irrespective of how many cores on the node are being used. ARCHER2 has 128 cores per node, and for the UM each MPI task and OpenMP thread is mapped to a separate core. So in this case we are running 10x16 (x 2 OMP threads) for a total of 320 cores, but are charged for 3 nodes (384 cores).

Try experimenting with different processor decompositions (E.g. 10x32, 16x32, etc)

• How do the timings compare to when you ran on 3 nodes?

You can come up with a performance vs processor count curve in this way which might be valuable if you are planning an experiment - it's also worth adding in the CU cost calculation when doing this. An example of this can be seen below:



Note: Running "under populated", i.e. with fewer than the total cores per node, gives access to more memory per parallel task.

Change the processor decomposition to run fully populated on 3 nodes with 2 OpenMP threads.

6.3 STASH

6.3.1 Exploring STASH

Navigate to *um* -> *namelist* -> *Model Input and Output* -> *STASH Requests and Profiles*. Look at the time profiles called TALLTS and T6H.

• What are they doing?

TALLTS says output on every timestep, T6H says output 6 hourly.

Look also at some of the other time, domain and usage profiles. The domain profiles determine spatial output and the usage profiles effectively specify a Fortran LUN (Logical Unit Number) on which the associated data is written.

Click on STASH Requests. Now change the time profile for all stash output whose Usage profile is UPC and Time profile is T6H. To do this, click on each diagnostic you wish to change and then click the time profile, a drop-down list should appear containing all the available time profiles. Select TALLTS. You can sort the STASH table to make it more convenient to make these changes. Click on the use_name column header to sort by usage profile.

6.3.2 STASH validation macro

Several Rose macros have been provided to help verify STASH setup. When you change STASH it is always recommended to run at least the validate macro. The *stash_testmask.STASHTstmskValidate* macro ensures that the STASH output requsted is valid given the science configuration of the app. To put this to the test run the STASH validation macro by selecting *stash_testmask.STASHTstmskValidate* from the list of available macros at the top of the STASH requests panel or alternatively it can be accessed from the *Metadata -> um* menu.

You should see several errors reported - it appears we have asked for diagnostics which are not available. This won't cause the model to fail, however, you could find these diagnostics in the list and switch them off by unchecking the "incl?" column, if you'd like to stop seeing this message.

Save and Re-run the suite.

The model should fail with an error message similar to the following:

STWORK: Number of fields exceeds reserved headers for unit 14

This means that the number of output fields exceeds the limit set for a particular stream (the default is 4096 fields); in this case the stream attached to unit 14. To find out what stream unit 14 is take a look in the fort6.pe000 file and search for "Unit 14". You should see that the file opened on unit 14 is <suite-id>a.pc19880901, so this is the pc stream. Back in rose edit for this suite look at the STASH usage profile for upc.

• What is the file ID of the failing output stream?

Now navigate to the window for this stream under *Model Input and Output -> Model Output Streams*. This defines the output stream. You should see confirmation of the base output file name to be *.pc*. Changing the reinitialisation frequency by modifying reinit_step and/or reinit_unit is the best way to fix this header problem. This tells the model to create new output files at a specified frequency, so individual files don't get massively large.

Note: If the model is only exceeding the numer of reserved headers by a small amount it is also possible to just increased the reserved_headers size. Overriding the size by a large amount and thus having large numbers of fieldsfile headers can be very inefficient for both runtime and memory. Therefore the recommended way is to change the periodic reinitialisation of the fieldsfiles.

Modify the reinitialisation frequency (you will need to experiment with the numbers) and run the model again. Take a look at the model output files. You should see that you have multiple *.pc19980901_* files.

6.3.3 Adding a new STASH request

Let's now try adding a new STASH request to the UM app.

Click the *New* button in the STASH Requests section. A window will appear in order for you to browse all available STASHmaster entries.

By default STASHmaster entries are grouped together by Section code. It is possible to group items by any of the STASHmaster codes using the Group drop down list. The *View* button contains options to display the STASHmaster entry values and/or the column titles with explanation text and to select which columns to show/hide.

Expand the *Gravity wave drag* section. Then change the view by selecting *View -> Show expanded value info*. Try out the other options in the *View* menu to see what effect they have.

Select a STASH item and click *Add* to add it to the list of STASH requests. In the STASH Requests panel click on the empty dom_name, tim_name and use_name fields of the new request and select appropriate profiles from the drop down lists. These lists are populated from the entries of the time, use and domain namelists.

Once you have added a new STASH request, you need to run a macro to generate an index for the namelist. To do so click on the *Macros* button, then select *stash_indices.TidyStashTransform*. A box will pop up listing the changes the editor is going to make, click *Apply*.

• Run the model. Did it work?

6.4 Change the dump frequency

Set the model run length to 6 hours.

Hint: Look in the *suite conf* -> *Run Initialisation and Cycling*.

Note: Hours are represented in the ISO 8601 standard as PT<num-hours>H (e.g. PT1H represents 1 hour). Days are represented as P<num-days>D (e.g. P10D represents 10 days)

Reset the STASH output for stream UPC to 6 hourly and the file reinitialisation frequency to daily.

Navigate to *um* -> *namelist* -> *Model Input and Output* -> *Dumping and Meaning*.

• What is the current dump frequency?

Set the dump frequency to 6 hours. *Run* the model.

• How much time was spent in DUMPCTL?

Set the dump frequency to 1 hour. *Run* the model.

• What happened to the time spent in DUMPCTL?

Important: It is important to understand that writing out model dumps, particularly at higher resolutions, takes up a large amount of time and contributes to the cost. You should think about how frequently you need to output model dumps when setting up your simulations.

6.5 Reconfiguration

Try to find out how to run the reconfiguration only.

Hint: Look in the *suite conf* section.

Try to find out where to request extra diagnostic messages for the reconfiguration output.

Run the reconfiguration only with extra diagnostic messages.

Look at the job. out file.

• Do you see a land-sea mask?

6.6 Setting up a suite to cycle

We mentioned in the presentations that the length of an integration will be limited by the time that a model is allowed to run on the HPC (see the ARCHER2 web pages for information about the time limits). Clearly this is no good for much of our work which may need to run on the machine for several months. Cylc and the UM allow for long integrations to be split up into multiple shorter jobs - this is called **cycling**.

Let's run the model for 1 day with 6 hour cycling:

- Set the Total run length to 1 day.
- Set the Cycling frequency to 6 hours.
- Set the Wallclock time to 10 minutes.
- Ensure that the model dump frequency is 6 hourly, in this case.

Save and Run the suite.

Note: The cycling frequency must be a multiple of the dump frequency.

The model will submit the first cycle and once that has succeeded you will see the following 3 cycles submitted and run.

Note: It is always wise, particularly when you plan to run a long integration, that you only run the first cycle initially so that you can check that the model is doing what you expect before committing to a longer simulation. It also enables you to determine how long it takes your model to run and thus be able to calculate an appropriate cycling frequency for your simulation.

6.7 Restarting a suite

Let's now extend this run out to 2 days. Change the Total run length to 2 days and Save the suite.

Having already run the first day we just want the suite to pick up where it left off and run the remaining day. To do this we *restart* the suite, by typing:

```
puma2$ rose suite-run --restart
```

The cylc GUI will pop up and you should see the run resuming from where it left off (i.e. from cycle point 19880902T0000Z).

FURTHER EXERCISES (2)

The exercises in this section are all optional. We suggest you pick and choose the exercises that you feel are most relevant to the work you are/will be doing.

Note: Use your copy of suite u-cc654 for these exercises unless otherwise specified.

7.1 Post-Processing (archive and transfer of model data)

When your model runs it outputs data onto the ARCHER2 /work disk (/projects on Monsoon2). If you are running a long integration and/or at high resolution data will mount up very quickly and you will need to move the data off of ARCHER2; for example to JASMIN. The post-processing app (postproc) is used within cycling suites to automatically *archive* model data and can be optionally configured to transfer the data from ARCHER2 to the JASMIN data facility. The app archives and deletes model output files, not only for the UM, but also NEMO and CICE in coupled configurations.

Let's try configuring your suite to archive to a staging location on ARCHER2:

• Switch on post-processing in window *suite conf* -> *Tasks*

The post-processing is configured under the *postproc* section:

• Select the *Archer* archiving system in window *Post Processing - common settings*.

A couple of new entries will have appeared in the index panel, *Archer Archiving* and *JASMIN Transfer*, identified with the blue dots.

You now need to specify where you want your archived data to be copied to:

• In the Archer Archiving panel set archive_root_dir to be /work/n02/n02/<userid>/ archive. The archive_name (suite id) will be automatically appended to this.

You will need to run the model for at least 1 day as archiving doesn't work for periods of less than 1 day. Change the run length and cycling frequency to be 1 day. This should complete in about 5 minutes so set the wallclock time to be 10 minutes.

Run the suite.

Once the run has completed go to the archive directory for this cycle (e.g. /nerc/n02/n02/<userid>/ <suiteid>/19880901T0000Z) and you should see several files have been copied over (e.g cc654a.pc19880901 00.pp).

Data files that have been archived and are no longer required by the model for restarting or for calculating means (seasonal, annual, etc) are deleted from the suite History Data directory. Go to the

History_Data directory for your suite and confirm that this has happened. This run is reinitialising the pc data stream every 6 hours and you should see that it has only removed data files for this stream up to 18:00hrs, the cc654a.pc19880901_18.pp file is still present. This file contains data for the hours 18-24 and would be required by the model in order to restart. Equally seasonal mean files would not be fully archived until the end of the year, after the annual mean has been created.

Note: The post-processing app can also be configured to transfer the archived data over to JASMIN. Details on how to do this are available on the CMS website: http://cms.ncas.ac.uk/wiki/Docs/PostProcessingApp

7.2 Using IO Servers

Older versions of the UM did not have IO servers, which meant that all reading and writing of fields files went through a single processor (pe0). When the model is producing lots of data and is running on many processors, this method of IO is very inefficient and costly - when pe0 is writing data, all the other processors have to wait around doing nothing but still consuming AUs. Later UM versions, including UM 10.5, have IO servers which are processors dedicated to performing IO and which work asynchronously with processors doing the computation.

Here's just a taste of how to get this working in your suite.

Set the suite to run for 1 day with an appropriate cycling frequency, then check that OpenMP is switched on as this is needed for the IO servers to work.

Hint: Search for openmp in the rose edit GUI

Navigate to *suite conf* -> *Domain Decomposition* -> *Atmosphere* and check the number of OpenMP threads is set to 2. Set the number of IO Server Processes to 8.

Save and then Run the suite.

You will see lots of IO server log files in ~/cylc-run/<suitename>/work/<cycle>/atmos_main which can be ignored for the most part.

Try repeating the *Change the dump frequency* experiment with the IO servers switched on - you should see much faster performance.

7.3 Writing NetCDF output from the UM

Until UM vn10.9, only fields-file output was available from the UM - bespoke NetCDF output configurations did exist but not on the UM trunk. The suite used in most of these Section 7 exercises is vn11.7, hence supports both fields-file and NetCDF output data formats.

7.3.1 Enable NetCDF

Make sure that IO Server Processes variable is set to 0.

Navigate to *um* -> *namelist* -> *Model Input and Output* -> *NetCDF Output Options* and set l_netcdf to true. Several fields will appear which allow you to configure various NetCDF options. For this exercise, leave them at their chosen values.

7.3.2 Set NetCDF Output Streams

Expand the *NetCDF Output Streams* section. A single stream - nc0 - already exists; select it to display its content. As a useful comaprison, expand the *Model Output Streams* section and with the middle mouse button select *pp0*. Observe that the only significant differences between pp0 and nc0 are the values of file_id and filename_base. Data compression options for nc0 are revealed if l_compress is set to true. NetCDF deflation is a computationally expensive process best handled asynchronously to computation and as yet not fully implemented through the UM IO Server scheme (but under active development.) For many low- to medium-resolution models and, depending precisely on output profiles, high-resolution models also, use of UM-NetCDF without IO servers still provides significant benefits over fields-file output since using it avoids the need for subsequent file format conversion.

Right-click on nc0 and select *Clone this section*. Edit the settings of the newly cloned section appropriately to make the new stream similar to pp1 (ie. edit filename_base and all the reinitialisation variables). It is sensible to change the name of the new stream from 1 to something more meaningful, nc1 for example (right click on 1, select *Rename a section*, and change ...nc(1) to ...nc (nc1)).

7.3.3 Direct output to the nc streams

Expand STASH Requests and Profiles, then expand Usage Profiles. Assign nc streams to usage profiles - in this suite, UPA and UPB are assigned to pp0 and pp1 respectively (where can you see this?). Edit these Usage profiles to refer to nc0 and nc1 respectively. Run the STASH Macros (if you need a reminder see Section 6), save the changes, and run the suite. Check that the NetCDF output is what you expected.

Try adding more nc streams to mimic the pp stream behaviour.

7.4 Running the coupled model

The coupled model consists of the UM Atmosphere model coupled to the NEMO ocean and CICE sea ice models. The coupled configuration used for this exercise is the UKESM Historical configuration with an N96 resolution for the atmosphere and a 1 degree ocean - you will see this written N96 ORCA1.

7.4.1 Checkout and run the suite

Checkout and open the suite u-cs147. The first difference you should see is in the naming of the apps; there is a separate build app for the um and ocean, called fcm_make_um and fcm_make_ocean respectively. Similarly there are separate apps for the atmost and ocean model settings, called um and nemo_cice.

Make the usual changes required to run the suite (i.e. set username, account code, queue). If you are following the tutorial as part of an organised training event, select one of the special queues, otherwise, select to run in the short queue.

Check that the suite is set to build the UM, Ocean, and Drivers as well as run the reconfiguration and model. *Run* the suite.

7.4.2 Exploring the suite

Whilst the suite is compiling and running which will take around 40 minutes, take some time to look around the suite.

- How many nodes is the atmosphere running on?
- How many nodes is the ocean running on?
- What is the cycling frequency?

The version of NEMO used in this suite (and most suites you will come across) uses the XML IO Server (XIOS) to wite its diagnostic output. XIOS runs on dedicated nodes (one node in this case). Running squeue will show three status entries corresponding to the Atmosphere, Ocean, and XIOS components of the coupled suite. XIOS is running in multiple-file mode with 6 servers.

• Can you see where the NEMO model settings appear?

Look under *Run settings* (namrun). The variables nn_stock and nn_write control the frequency of output files.

• How often are NEMO restart files written?

Hint: The NEMO timestep length is set as variable rn_rdt

Now browse the CICE settings.

• Can you find what the CICE restart frequency is set to?

NEMO, CICE and XIOS are developed separately from the UM, and you should have seen that they work in very different ways. See the following websites for documentation:

- http://oceans11.lanl.gov/trac/CICE
- http://www.nemo-ocean.eu/
- https://forge.ipsl.jussieu.fr/ioserver

7.4.3 Output files

Log files

NEMO logging information is written to:

~/cylc-run/<suitename>/work/<cycle>/coupled/ocean.output

CICE logging information is written to:

~/cylc-run/<suitename>/work/<cycle>/coupled/ice_diag.d

If the model fails some error messages may also be written to the file ~/cylc-run/<suitename>/work/<cycle>/coupled/debug.root.01 or debug.root.02

When something goes wrong with the coupled model it can be tricky to work out what has gone wrong. NEMO errors may not appear at the end of the file but will be flagged with the string E R R O R.

Restart files

Restart files go to the subdirectories NEMOhist and CICEhist in the standard data directory ~/cylc-run/<suitename>/share/data/History_Data.

Diagnostic files

Diagnostic files are left in the ~/cylc-run/<suitename>/work/<cycle>/coupled/ directory.

CICE files start with <suitename>i. Once your suite has run you should see the following CICE file (and more):

```
archer$ ls cel19i* cel19i.10d.1850-01-10.nc
```

NEMO diagnostic files are named <suitename>o*grid_[TUVW] *. To see what files are produced, run:

```
archer$ ls cel19o*grid*
```

In this case each XIOS IO server writes to a separate file. To concatenate these into a global file use the rebuild_nemo tool, e.g.:

```
archer$ rebuild_nemo ce119o_1d_18500101_18500110_grid_T 6
```

Note: The coupled atmos-ocean model setup is complex so we recommend you find a suite already setup for your needs. If you find you do need to modify a coupled suite setup please contact NCAS-CMS for advice.

7.5 Running the Nesting Suite

The Nesting Suite drives a series of nested limited area models (LAM) from a global model. It allows the user to specify the domains and it then automatically creates the required ancillary files and lateral boundary condition files.

7.5.1 Checkout and run the suite

Checkout and open the suite u-ce122. There are a number of tasks for creating ancillary files (ancil_* and ants_*). The global model set up is in glm_um and the LAMs are in um. The task um-createbc creates the lateral boundary condition files.

Under *suite conf* -> *jinja2:suite.rc* are the main panels for controlling the Nesting Suite. Make the usual changes required to run the suite (i.e. set username, account code, queue).

If following the tutorial as part of an organised training event, select one of the special queues, otherwise, select the short queue.

Run the suite.

This particular suite has a global model and one limited area model. It should complete in about 45 - 60 minutes.

7.5.2 Exploring the Suite

The Driving Model set up panel allows the user to specify the resolution of the global model and the number of nested regions.

The *Nested Region 1* set up panel specifies the latitude and longitude of the centre of the first nested region. All the other limited area models have the same centre.

A useful way to get this information is to use Google Maps. Find the place you want as a centre and then press control-left mouse and a little window with the latitude and longitude appears.

• Can you find out where the first LAM is located?

Hint: Look at the orography file output during the ancillary creation.

The *resolution 1* set up panel specifies the grid and the run length.

The *Config 1* set up panel specifies the science configuration to be run. Each LAM can have multiple science configurations.

7.5.3 Initial Data

The initial data for the global model is in share/cycle/<cycle time>/glm/ics

The initial data for the first LAM is in $share/cycle/cycle time>/Regn1/resn_1/RA1M/ics$

The RA1M is the name you gave to the first science configuration.

The LBCs for the first LAM are in share/cycle/<cycle time>/Regn1/resn_1/RA1M/lbcs.

7.5.4 The ancillary files

These are in share/data/ancils/Regn1/resn_1

7.5.5 The output files

The global model output is in share/cycle/<cycle time>/glm/um. This also contains the data for creating the LBC files (umglaa_cb*) for the first LAM.

Diagnostic files can be found under work/cycle time> in an application directory. For example, the region1 forecast diagnostics is in work/cycle time>/Regn1_resn_1_RA1M_um_fcst_000. This will include the pe_output files.

The output for the first LAM is in share/cycle/<cycle time>/Regn1/resn_1/RA1M/um.

7.5.6 Further Information

This has been a very brief overview of the functionality of the Nesting Suite. The Nesting Suite is developed and maintained by Stuart Webster at the Met Office. He has a web page all about the Nesting Suite at https://code.metoffice.gov.uk/trac/rmed/wiki/suites/nesting. This includes a more detailed tutorial.

SECTION

EIGHT

ROSE/CYLC EXERCISES

8.1 Differencing suites

Currently there is no Rose tool to difference two suites. Since a suite consists of text files it is simply a matter of making sure all the Rose configuration files are in the common format by running rose configuration each suite and then running diff.

We will difference your copy of the GA7.0 suite with the original one:

```
puma2$ cd ~/roses
puma2$ rosie checkout u-cc654
puma2$ rose config-dump -C u-cc654
puma2$ rose config-dump -C <your-suitename>
puma2$ diff -r u-cc654 <your-suitename>
```

• Are the differences what you expected?

8.2 Graphing a suite

When developing suites, it can be useful to check what the run graph looks like after jinja evaluation, etc.

The GA7.0 suite that we have been working with is very simple so we shall graph a nesting suite which is more complex. To do this without running the suite:

```
puma2$ rosie checkout u-ce122
puma2$ cd ~/roses/u-ce122
puma2$ rose suite-run -l --name=u-ce122 # install suite in local cylc db only
puma2$ cylc graph u-ce122 # view graph in browser
```

A window containing the graph of the suite should appear. By default tasks in the same family are grouped together. Click the *Ungroup all families* button at the top of the window to expand the graph to view all tasks within this suite.

8.3 Exploring the suite definition files

Change to the ~/roses/<suite-id> directory for your copy of u-cc519.

Open the suite.rc file in your favourite editor.

Look at the [scheduling] section. This contains some Jinja2 variables (BUILD & RECON) which allow the user to select which tasks appear in the dependency graph. The dependency graph tells Cylc the order in which to run tasks. The fcm_make and recon tasks are only included if the BUILD and RECON variables are set to true. These variables are located in the rose-suite.conf and can be changed using the rose edit GUI or by directly editing the rose-suite.conf file. When you run a suite, a processed version of the suite.rc file, with all the Jinja2 code evaluated, is placed in your suite's cylc-run directory.

• Take a look at the suite.rc.processed file for your suite.

Hint: Go to directory ~/cylc-run/<suite-id>.

- Change the values of BUILD and RECON and re-run your suite.
- Look at the new suite.rc.processed file. Can you see how the graph has changed?

Make sure that you leave the suite with BUILD=false before continuing.

As we saw earlier when changing the path to the start dump, some settings can't be changed through the rose edit GUI. Instead you have to edit the suite definition files directly.

- Can you find where the atmos processor decomposition is set for this suite?
- Change atmos processor decomposition to run on 2 nodes. Run the suite.
- Did it work? If not, what error message did you get?

Hint: Look in the usual job.out/job.err or it may be in the job-activity.log file.

You will get an error if the processor decomposition of the model does not match the number of tasks and nodes requested by Slurm. For details on the Slurm batch system on ARCHER2 see: https://docs.archer2.ac.uk/user-guide/scheduler/).

In the [[atmos]] [[[directives]]] section, set --nodes=2 and --ntasks=256 to tell the Slurm scheduler that you require 2 nodes and a total of 256 MPI tasks.

- The suite should run this time. Did it run on 2 nodes as requested?
- How much walltime has been requested for the reconfiguration?

Now take a look at the suite.rc file for your other suite (the one copied from u-cc654). See how it differs. This one is set up to run on multiple platforms.

- Can you see the more complex dependency graph?
- Why do you not need to adjust the Slurm directives to change the processor decomposition in this suite?
- Can you see where to change the reconfiguration walltime for this suite?

This has just given you a very brief look at the suite definitions files. More information can be found in the cylc documentation: https://cylc.github.io/cylc-doc/7.8.8/html/index.html

8.4 Starting a suite in "held" mode

This allows you to trigger the running of tasks manually.

To start a suite in held mode add -- --hold to the end of the rose suite-run command:

```
puma2$ rose suite-run -- --hold
```

The first — tells Rose that all subsequent options should be passed on to Cylc. This is why the hold option should be added to the end of the command, after any Rose options. Once the suite has started all tasks will be in a held state. It is then possible to select which tasks are run by right clicking on a task in the Cylc GUI and manually triggering it or resetting its state.

Try doing this as a way to run the reconfiguration only in one of your suites.

8.5 Discovering running suites and the multi-suite monitor GUI

Suites that are currently running can be detected with command line or GUI tools:

Submit 2 of your suites. It doesn't matter what tasks they are running for this exercise; compilation, recon or model run.

Now try running the command cylc scan. This lists your currently running suites. For example:

```
puma2$ cylc scan
u-af140 ros@localhost:7770
u-ag761 ros@localhost:7776
```

There is also a multi-suite monitor GUI, which allows you to monitor the states of all suites you have running in one window. Try running the command:

```
puma2$ cylc gscan &
```

Double clicking on a suite in gscan GUI opens the Cylc GUI window, which you will be very familiar with by now. For each suite open the Cylc GUI window and stop the suite by going to Control > Stop Suite, selecting $Stop \ after \ killing \ active \ tasks$ and clicking Ok.

8.6 Adding a new app to a suite

A Rose application or "Rose app" is a Rose configuration for running an executable command, encapsulating details such as scripts, programs and settings.

To add a new app to a suite, we first create a directory to hold the app files. The main details are specified in a configuration file rose-app.conf. We may also specify some metadata to tell the general user what inputs to the task mean (this goes under a meta/sub-directory or we may reference some standard metadata held elsewhere). Any scripts or executables needed by the new app can be added into an app bin/directory. General scripts that aren't specific to the app should go in the *suite* bin/directory.

Remember to fcm add any new files that you add to the suite so they will be added to the repository when you next commit.

In order to actually run the app, we need to add a new "task" to the suite which involves editing the suite configuration file suite.rc. We need to specify 3 things:

- 1. How the new task relates to other tasks, specifically, which task will trigger it and which task will follow it;
- 2. What the task will run (i.e which app); and
- 3. How the task will run (i.e. which computer and the resources it will need).

In this example, we will add an app that prints Hello World, which will execute after the reconfiguration and before the main model. We will add the app to your copy of u-cc654.

8.6.1 Create the Rose application directory

Make sure the Rose edit GUI for your suite is closed. cd into the suite app/ directory and create a new directory called new_app

```
puma2$ cd ~/roses/<SUITEID>/app
puma2$ mkdir new_app
```

8.6.2 Create the Rose app configuration file

Change into the new_app directory and create a blank app configuration file called rose-app.conf:

```
puma2$ touch rose-app.conf
```

Start the Rose editor (remember you need to be in the top level of the suite directory). You should now see the new application listed in the left hand panel. At this point it is an empty application and is not integrated into the task chain. Click on *new_app* to load the app and then the little triangle to the left of *new_app* to expand its contents.

Tip: You may need to select *View > View Latent Pages* to see the little triangle

Everything is greyed out. Click on *command* to see the command page and then click the + sign next to command default. Again you may need to select *View -> View Latent Variables* to see it. Select *add to configuration* to add a command to the application. Enter echo "Hello World" in the command default box. *Save* this and then have a look at the contents of the rose-app.conf file to see the effect.

8.6.3 Add a new task to the suite definition

In order to execute the app, we need to add a new task to the suite workflow. This task executes our new application on a machine that we specify. In this instance we are adding the new task between the reconfiguration and the model run, and the task will be run on ARCHER2 in the serial queue.

To set this up, edit the suite.rc file. Under,

and change it to

```
{% set INIT_GRAPH = INIT_GRAPH ~ ' => hello => atmos_main' if TASK_RUN else_
→INIT_GRAPH %}
```

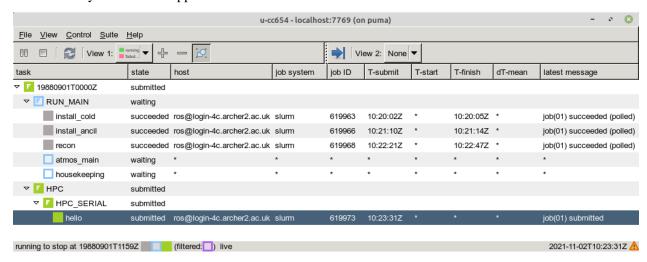
This puts the task hello in the right place in the task list.

The next step is to add a definition for the new task. To tell Rose to use one of the apps contained in the suite, we set the environment variable ROSE_TASK_APP in the task definition. General task definitions go in the suite.rc file and the definitions specific to ARCHER2 in the site/archer2.rc file. The queuing system is specific to the host being run on, and there is already a definition for the ARCHER serial queue environment [[HPC_SERIAL]] that we can make use of. To run the new application on ARCHER2 in the serial queue and give it two minutes to complete, add the following lines to the suite.rc after the definition for [[recon]]:

```
[[hello]]
  inherit = HPC_SERIAL
  [[[environment]]]
    ROSE_TASK_APP = new_app
  [[[job]]]
    execution time limit = PT2M
```

8.6.4 Running the new app

We are now ready to go. *Run* the suite. Look at the task graph: recon and atmos_main are there, but a new hierarchy of tasks has appeared.



Notice that atmos_main no longer runs after the reconfiguration, but our new task hello does and when that has completed, atmos_main starts. The output from the hello task can be found in the cylc output directory: log/job/19880901T0000Z/hello/NN/job.out.

8.6.5 Extending the app to run a script

A more complex application might involve the execution of a script. To do this we would replace the contents of the command default box with the name of the script. Then place the script in the app bin/directory.

Now create a bin/directory under new_app/ and cd into it. Create a file called hello.sh with the contents,

```
#!/bin/bash
echo "Hello, $1!"
```

We will allow the user to select from a variety of planets and say hello. Make it an executable script:

```
chmod +x hello.sh
```

Then we can say ./hello.sh Jupiter to get it to print "Hello, Jupiter!".

Right click on the greyed out *new_app* -> *env* in the index panel and click + *Add env*. *Save*, then select *new_app* -> *env* to view the env page, right click on the blank page and select *Add blank variable*. Two boxes appear: enter PLANET in the first and Jupiter in the second. This adds an environment variable called PLANET and sets it to Jupiter.

Now change the command from echo "Hello, World" to hello.sh \${PLANET}.

8.6.6 Testing and Running

The app can be tested in isolation by changing into the new_app/ directory and executing,

```
rose app-run
```

This should produce output similar to:

```
ros@puma2$ rose app-run
[INFO] export PATH=/home/ros/roses/u-cc654/app/new_app/bin:/home/fcm/rose-
→2016.11.1/bin:/usr/local/python/bin:
...
[INFO] export PLANET=Jupiter
[INFO] command: hello.sh ${PLANET}
Hello, Jupiter!
```

and also a file rose-app-run.conf, which can be deleted.

Now Run the suite.

8.6.7 Rose Metadata

Metadata can be used to provide information about settings in Rose configurations. It is used for documenting settings, performing automatic checking and for formatting the rose edit GUI. Metadata can be used to ensure that configurations are valid before they are run.

Metadata for many standard applications, such as um-atmos, fcm_make are all stored centrally on PUMA2 in ~fcm/rose-meta. Have a look at this directory.

For our example there are currently no restrictions on the variable PLANET. We will now add some metadata to help the user understand what the variable PLANET is and what values it is limited to.

Rose provides some tools to quickly guess at the metadata where there is none. Create a directory $meta/under new_app/$. Then execute the command,

```
rose metadata-gen
```

This creates a file rose-meta.conf in the meta/ directory. It just says that there is an evironment variable called PLANET, but it does not know much about it. Edit this file and add the following lines after [env=PLANET]:

```
description=The name of the planet to say hello to.
values=Mercury, Venus, Earth, Mars, Jupiter, Saturn, Uranus, Neptune
help=Must be a planet bigger than Pluto - see https://en.wikipedia.org/wiki/
Solar_System
```

Now go back to the Rose GUI and select *Metadata* > *Refresh Metadata*. Once the metadata has reloaded, go to the *new_app* -> *env* panel. The entry box for PLANET has changed into a drop down list. Pluto is not allowed, presumably because the code cannot handle tiny planets. Right click on the cog next to Planet and select *info* to see the description and allowed values.

8.6.8 References

A fuller discussion of Rose metadata can be found at https://metomi.github.io/rose/2019.01.8/html/tutorial/rose/metadata.html.

Designing a new application may seem a daunting process, but there are numerous existing examples in suites that you can try to understand. For further details, see the Rose documentation at https://metomi.github.io/rose/2019.01.8/html/tutorial/rose/applications.html. There are a collection of built-in applications that you can use for building, testing, archiving and housekeeping - see https://metomi.github.io/rose/2019.01.8/html/api/rose-built-in-applications.html.

POST PROCESSING

This is simply a very basic introduction to some of the more widely used useful tools for viewing, checking, and converting UM input and output data. The tools described below all run on the ARCHER2 login nodes.

9.1 xconv

9.1.1 View data

On ARCHER2 go to the output directory of the global job that you ran previously (the one copied from u-cc654). Run xconv on the file ending with, for example, da19880901_04. This file is an atmosphere start file - this type of file is used to restart the model from the time specified in the file header data.

In the directory above is a file whose name ends in .astart; run a second instance of xconv on this file. This is the file used by the model to start its run - created by the reconfiguration program in this case.

The xconv window lists the fields in the file, the dimensions of those fields (upper left panel), the coordinates of the grid underlying the data, the time(s) of the data (upper right panel), some information about the type of file (lower left panel), and general data about the field (lower right panel.)

Both files have the same fields. Double click on a field to reveal its coordinate data. Check the time for this field (select the "t" checkbox in the upper right panel).

Plot both sets of data - click the Plot Data button.

View the data - this shows numerical data values and their coordinates and can be helpful for finding spurious data values.

9.1.2 Convert UM fields data to netCDF

Select a single-level field (one for which nz=1), choose *Output format* to be *Netcdf*, enter an "Output file name", and select *Convert*. Information relevant to the file conversion will appear in the lower left panel.

Use xconv to view the netcdf file just created.

9.2 uminfo

You can view the header information for the fields in a UM file by using the utility uminfo - redirect the output to a file or pipe it to less:

```
archer2$ uminfo <one-of-your-fields-files> | less
```

The output from this command is best viewed in conjunction with the Unified Model Documentation Paper F3 which explains in depth the various header fields.

9.3 Mule

Mule consists of a Python API for reading and writing UM files and a set of UM utilities. This section introduces you to some of the most useful UM utilities. Full details of Mule can be found on the MOSRS: https://code.metoffice.gov.uk/doc/um/index.html

Before running the mule commands you will need to load the python environment on ARCHER2 by running:

```
archer2$ module load cray-python
```

9.3.1 mule-pumf

This provides another way of seeing header information, but also gives some information about the fields themselves. Its intended use is to aid in quick inspections of files for diagnostic purposes.

Run mule-pumf on the start file - here's a couple of examples on one of Ros' files:

• Can you see what the difference is in the output of these 2 commands?

Take a look at the man page (mule-pumf -h) and experiment with some of the other options

9.3.2 mule-summary

This utility is used to print out a summary of the lookup headers which describe the fields from a UM file. Its intended use is to aid in quick inspections of files for diagnostic purposes.

Run mule-summary on the start file again.

9.3.3 mule-cumf

This utility is used to compare two UM files and report on any differences found in either the headers or field data. Its intended use is to test results from different UM runs against each other to investigate possible changes. Note, differences in header information can arise even when field data is identical. Try out the following:

- Run mule-cumf on the two start files referred to above (in the "View data" section). You may wish to direct the output to a file.
- Run the same command but with the --summary option. This, as the name suggests, prints a much shorter report of the differences.
- Run mule-cumf on a file and itself.
- View the help page with mule-cumf -h to find view all the available options.

9.4 um-convpp

We have mentioned in the presentations the PP file format - this is a sequential format (a fields file is random access) still much used in the community. PP data is stored as 32-bit, which provides a significant saving of space, but means that a conversion step is required from a fields file (64-bit). The utility to do this is called um-convpp. um-convpp converts directly from 64-bit files produced by the UM to 32-bit PP files. You must, however, make sure you are using a version 10.4 or greater - you can check that you are using the right one by typing which um-convpp.

Set the stack size limit to unlimited, and add the path to um-convpp to your environment - you can also add this to your ~/.profile so it is available everytime you log in.

```
archer2$ ulimit -s unlimited archer2$ export PATH=$UMDIR/vn11.2/cce/utilities:$PATH

Run um-convpp on a fieldsfile (E.g cc654a.pc19880901_00)

archer2$ cd /home/n02/n02/ros/cylc-run/u-cc654/share/data/History_Data archer2$ um-convpp cc654a.pc19880901_00 cc654a.pc19880901_00.pp

archer2$ ls -l cc654a.pc19880901*
-rw-r--r-- 1 ros n02 26447872 Nov 2 10:36 cc654a.pc19880901_00
-rw-r--r-- 1 ros n02 20372768 Nov 2 10:47 cc654a.pc19880901_00.pp
-rw-r--r-- 1 ros n02 26476544 Nov 2 10:36 cc654a.pc19880901_06
```

Note the reduction in file size. Now use xconv to examine the contents of the PP file.

9.5 cfa

There is an increasing use of python in the community and we have, and continue to develop, python tools to do much of the data processing previously done using IDL or MATLAB and are working to extend that functionality. cfa is a python utility which offers a host of features - we'll use it to convert UM fields file or PP data to CF-compliant data in NetCDF format. You first need to set the environment to run cfa:

```
archer2$ export PATH=/home/n02/n02/dch/cf-analysis/bin:$PATH archer2$ cfa -i -o cc654a.pc19880901_00.nc cc654a.pc19880901_00.pp
```

Try viewing the NetCDF file with xconv.

cfa can also view CF fields. It can be run on PP or NetCDF files, to provide a text representation of the CF fields contained in the input files. Try it on a PP file and its NetCDF equivalent, e.g.

```
archer2$ cfa -vm cc654a.pc19880901_00.pp | less
Field: long_name: HEAVYSIDE FN ON P LEV/UV GRID (ncvar%UM_m01s30i301_vn1100)
              _____
              : long_name:HEAVYSIDE FN ON P LEV/UV GRID(time(5), air_
\rightarrowpressure(17), latitude(145), longitude(192))
Cell methods : time: point
              : time(5) = [1988-09-01T00:00:00Z, ..., 1988-09-01T03:59:59Z]
Axes
→360_day
              : air_pressure(17) = [1000.0, ..., 10.0] hPa
               : latitude(145) = [-90.0, ..., 90.0] degrees_north
               : longitude(192) = [0.0, ..., 358.125] degrees_east
Field: long_name: VORTICITY 850 (ncvar%UM_m01s30i455_vn1100)
             : long_name: VORTICITY 850 (time(5), latitude(145),
\rightarrowlongitude (192))
Cell methods
              : time: point
              : air_pressure(1) = [-1.0] hPa
Axes
              : time(5) = [1988-09-01T00:00:00Z, ..., 1988-09-01T03:59:59Z]_
→360_day
              : latitude(145) = [-90.0, ..., 90.0] degrees_north
               : longitude(192) = [0.0, ..., 358.125] degrees_east
```

9.6 CF-python CF-plot

Many tools exist for analysing data from NWP and climate models and there are many contributing factors for the proliferation of these analysis utilities, for example, the disparity of data formats used by the authors of the models, and/or the availability of the underlying software. There is a strong push towards developing and using python as the underlying language and CF-netCDF as the data format. CMS is home to tools in the CF-netCDF stable - here's an example of the use of these tools to perform some quite complex data manipulations. The user is insulated from virtually all of the details of the methods allowing them to concentrate on scientific analysis rather than programming intricacies.

• Set up the environment and start python.

```
archer2$ export PATH=/home/n02/n02/dch/cf-analysis/bin:$PATH
archer2$ python
>>>
```

We'll be looking at some AIRS satellite-retrieved temperature data over sea.

• Import the cf-python library

```
>>> import cf
```

• Read in the AIRS data files

```
>>> f = cf.read('~dch/UM_Training/ta_mon_AIRS-1-0_BE_gn_*.nc')[0]
```

Inspect the file contents with different amounts of detail

```
>>> f
>>> print(f)
>>> f.dump()
```

Note that the ten AIRS files (one for each year) are automatically aggregated into one field.

• Read in another field produced by a GCM, this has a different latitude/longitude grid to the AIRS data

```
>>> g = cf.read('~dch/UM_Training/tas_Amon_HadGEM3-GC3-1_hist-1p0_

+r3i1p1f2_gn_185001-201412.nc')[0]

>>> print(g)
```

• Regrid the observed AIRS data (f) to the grid of the model field (g) over Europe. Use the "conservative" regridding method that preserves area integrals

Note that the latitude and longitude dimensions are now shorter in length.

• Average the regridded field over June-August for each year

Note that the time axis is now of length 1.

• Import the cfplot visualisation library

```
>>> import cfplot
```

• Make a default contour plot of the regridded observed data, £ at the 1000 hPa level

```
>>> f = f.subspace(Z=cf.eq(1000, 'hPa'))
>>> cfplot.con(f)
```

• Make a "blockfill" plot of the regridded observed data, f

```
>>> cfplot.con(f, blockfill=True)
```

• Make a default contour plot of the model data, g for its first time:

```
>>> g = g.subspace(T=[0])
>>> cfplot.con(g)
```

• Make a "blockfill" plot of the model data, q, restricting the view to over Europe

```
>>> cfplot.mapset(lonmin=-10, lonmax=40, latmin=25, latmax=70)
>>> cfplot.con(g, blockfill=True)
```

• Write out the regridded data to disk

```
>>> cf.write(f, 'obs_temperature_Europe_JJA_2003-2010.regridded.nc')
```



SECTION

TEN

APPENDIX A: USEFUL INFORMATION

10.1 UM output

ARCHER2 job output directory:

The standard output and error files (job.out & job.err) for the compile, reconfiguration and run are written to the directory:

```
~/cylc-run/<suite-id>/log/job/<cycle>/<app>
```

ARCHER2 model output:

By default the UM will write all output (e.g. processor output and data files) to the directory it was launched from, which will be the task's **work** directory. However, all output paths can be configured in the GUI and in practice most UM tasks will send output to one or both of the suite's **work** or **share** directories:

```
~/cylc-run/<suitename>/work/1/atmos
~/cylc-run/<suitename>/share/data
```

10.2 ARCHER2 architecture

ARCHER2 has two kinds of processor which we commonly use - they have several names, but roughly speaking they are the service processors (several nodes worth) sometimes referred to as the front end, and the compute processors (many many nodes worth) sometimes referred to as the back end. We login to the front end and build the model on the front end. We run the model on the back end. You wouldn't generally have an interactive session on the back end and will submit jobs there through the batch scheduler (slurm).

The UM infrastructure recognises this architecture and will run tasks in the appropriate place.

If you are doing any post-processing or analysis you may wish to submit your own parallel or serial jobs. Intensive interactive tasks should be run on the post-processor nodes (note. these will be available when the full system is in service.)

Consult the ARCHER2 documentation for details (See www.archer2.ac.uk).

10.3 ARCHER2 file systems

ARCHER2, in common with some other HPC systems, such as MONSooN, has (at least) two file systems which have different properties, different uses, different associated policies and different names. On ARCHER2 there are /home and /work. The /home file system is backed up regularly (only for disaster recovery), has relatively small volume, can efficiently handle many small files, and is where we recommend the UM code is saved and built. The /home system can not be accessed by jobs running on the compute processors.

The /work file system is optimized for fast parallel IO - it doesn't handle small files very efficiently. It is where your model will write to and read from.

10.4 ARCHER2 node reservations

In normal practice you will submit your jobs to the parallel queue on ARCHER2; the job scheduler will then manage your job request along with all those from the thousands of other users. For this training course, we will be using processor Reservations, whereby we have exclusive access to a prearranged amount of ARCHER2 resource meaning that you will not need to wait in the general ARCHER2 queues. Reservations are specified by a reservation code - e.g. n02-training_266. As an ARCHER2 user you can make a reservation so that you have access to the machine at a time of your choosing - reservations incur a cost overhead (50%), so best used when you are sure you need them.

10.5 Useful Rose commands

```
rose suite-run
     Run a suite.
rose suite-run --new
     Clear out any existing cylc-run directories for this suite and then run it. Take care when using
     this option as it deletes all files from any previous runs of the suite.
rose suite-run --no-log-archive
     Do not archive (tar-gzip) old log directories.
rose suite-run --restart
     Restart the suite from where it finished running previously
rose suite-run [--restart] -- --hold
     Hold (don't run tasks) immediately on running or restarting the suite
rose suite-shutdown
     Shutdown (stop) a running suite.
rose sgc
     Launch the Cylc GUI for a running suite.
rose suite-scan
```

Scan for any running suites. This is useful when you've shutdown the cylc GUIs and wish to quickly see what suites you still have running.

For more information on all these commands and more see the Rose and Cylc documentation or run rose command --help (E.g. rose suite-run --help) to view the man pages.

10.6 Problems shutting down suites

Types of shutdown

By default when you try to shutdown a suite, cylc will wait for any currently running tasks to finish before stopping, which may not be what you want to do. You can also tell cylc to kill any active processes or ignore running processes and force the suite to shutdown anyway. The latter is what you will need to do if the suite has got stuck:

```
rose suite-shutdown -- --now
```

To access these options in the cylc GUI, go to "Control" -> "Stop Suite". See also rose help suite-shutdown for further details.

Forcing shutdown

Sometimes after trying to shutdown a suite, it will still appear to be running.

First make sure you have used the correct shutdown command and aren't waiting for any unfinished tasks (see above). It can take cylc a little while to shut down everything properly, so be patient and give it a few minutes.

If it still appears to be running (for example you get an error when you try to re-start the suite), you may have to do the following:

• Manually kill the active processes:

Get a list of processes associated with the suite. For example, for suite u-cn134 you would run:

This gives a list of processes. The number in the 4th column is the process-id. Use this to kill each of the processes, eg:

```
kill -9 15688
```

- Try restarting the suite.
- If that still doesn't work you may also need to delete the contact file:

```
This lives in ~/cylc-run/<suiteid>/.service directory. For example: rm ~/cylc-run/u-cn134/.service/contact
```

SECTION

ELEVEN

APPENDIX B: SSH FAQS

This Sections provides instructions for some common ssh tasks. If you have any problems, contact a member of the CMS team.

11.1 Using an existing ssh agent

If you already have an ssh-agent set up on PUMA2, you can use this one to connect to your ARCHER2 training account. Conversely, after the course you may wish to use the keys you set up for own Archer account.

You can copy your ssh key over to Archer using the ssh-copy-id script.

First you need to find the name of the public key in your .ssh directory.

```
puma2$ cd ~/.ssh
puma2$ ls
environment.puma2.archer2.ac.uk id_rsa id_rsa.pub known_hosts ssh-setup
```

The public key ends with .pub and will usually be called id_rsa.pub or id_dsa.pub.

Now run the script to copy the key to your ARCHER2 account, making sure to use the correct name for your key:

```
puma2$ ssh-copy-id -i ~/.ssh/id_rsa.pub <archer-username>@login.archer2.ac.uk
```

You will be prompted for your Archer password.

If successful, you should now be able to login to Archer without a password. If you are prompted for a passphrase you need to re-start your agent - see below.

11.2 Restarting your ssh agent

Normally your ssh agent persists even when you log out of puma2. However, from time to time it can vanish.

If you are prompted for your passphrase, this means the ssh agent has stopped for some reason. The agent *should* have been re-initialised when you logged into PUMA2, but you will need to re-associate your ssh keys to the agent.

To do so, run:

```
puma2$ ssh-add
```

If successful this will prompt for your passphrase:

```
Enter passphrase for /home/<puma2-username>/.ssh/id_rsa_archerum:
```

Sometimes this step will fail with the following error:

```
Could not open a connection to your authentication agent.
```

In this case, the agent is not running. Usually this is beacuse of an environment file. Delete the following:

```
puma2$ rm ~/.ssh/environment.puma2.archer2.ac.uk
```

Then log out of puma2 and back in again. You should hopefully see a message similar to:

```
Initialising new SSH agent...
```

And you should now be able to run ssh-add successfully.

11.3 Regenerating your ssh keys

If you have forgotten your passphrase you will need to regenerate your ssh keys. Before doing so, you will need to tidy up the old keys otherwise the ssh agent can get itself confused.

Go to your .ssh directory, and look at the files:

```
puma2$ cd ~/.ssh
puma2$ ls
environment.puma2.archer2.ac.uk id_rsa id_rsa.pub known_hosts ssh-setup
```

Delete the public and private keys. These will normally be named id_rsa and id_rsa.pub, or id_dsa and id_dsa.pub.

You should also delete the environment.puma2.archer2.ac.uk file:

```
puma2$ rm id_rsa id_rsa.pub environment.puma2.archer2.ac.uk
```

Next check if you have an agent running:

```
puma2$ ps -flu <puma2-username> | grep ssh-agent
```

If you have an agent running, one or more lines like the following will be returned:

```
15658 ? 00:00:00 ssh-agent
```

The number in the first column is the process-id, pass this to the kill command to stop the process, for example:

```
puma2$ kill -9 15658
```

You can now start again, following the ssh set up instructions.