UNIVERSITY OF CAMBRIDGE
Yusuf Hamied
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How to do virtually everything with UKCA

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- What is the Unified Model, and how is code developed for it?
- What do I mean by *“virtually”*?
- What do I mean by *“virtually everything”*?
- What do I mean by *“everything”*?

What is the Met Office Unified Model?

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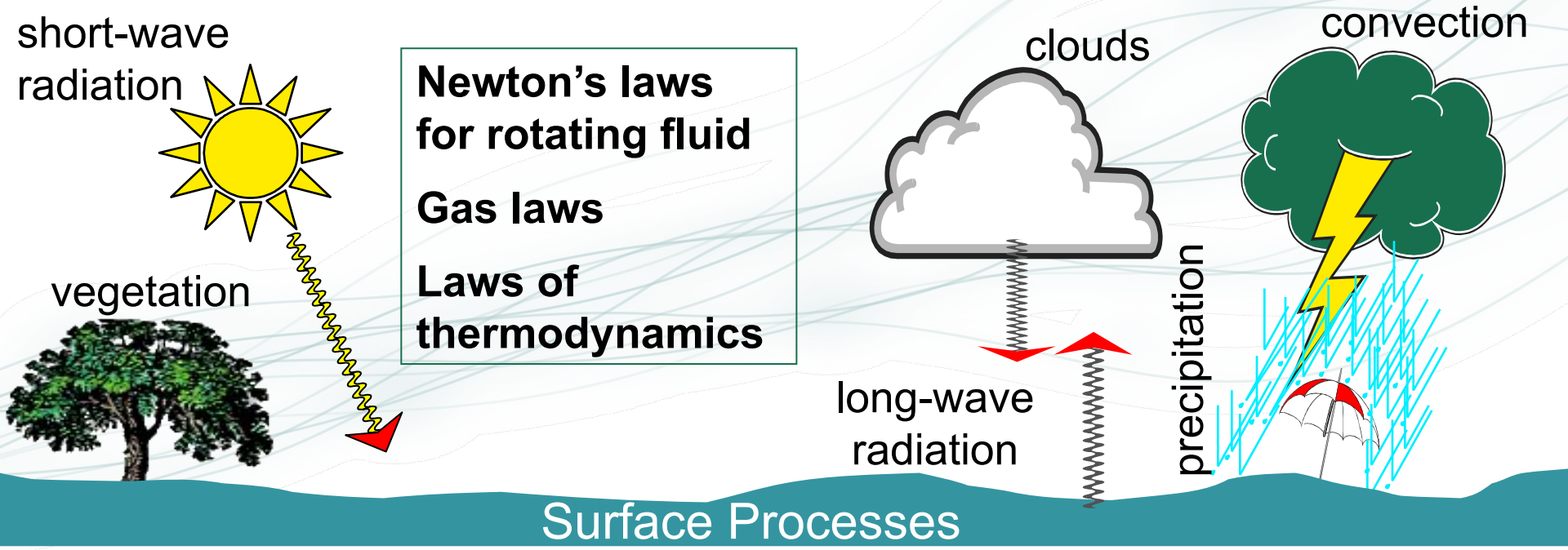
Atmospheric Modelling: integrating our knowledge of atmospheric behaviour forward in time



- The challenge: To reproduce the behaviour of (hazardous) weather systems

Unified Model

Brown et al. (2013)

- Operational forecasts
  - Mesoscale (resolution approx. 4km, 1.5km)
  - Global scale (resolution approx. 17km)
- Seasonal predictions
  - Resolution approx. 60km
- Global and regional climate predictions
  - Resolution around 120km
  - Run for 10-100-… years
- Research mode
  - Resolution 1km - 10m

> 25 years old

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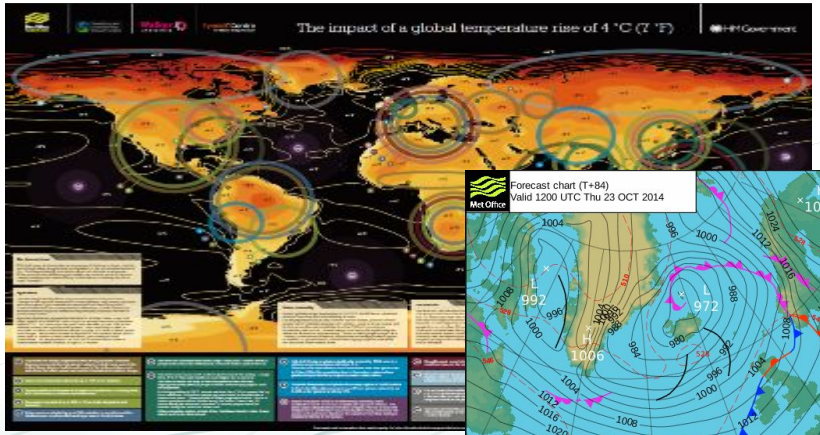
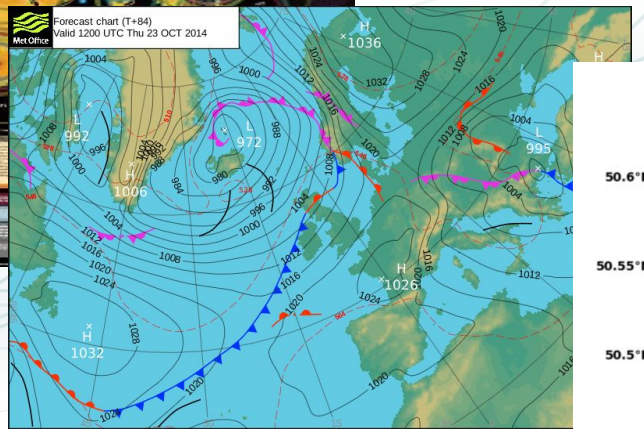
The consequence of unification

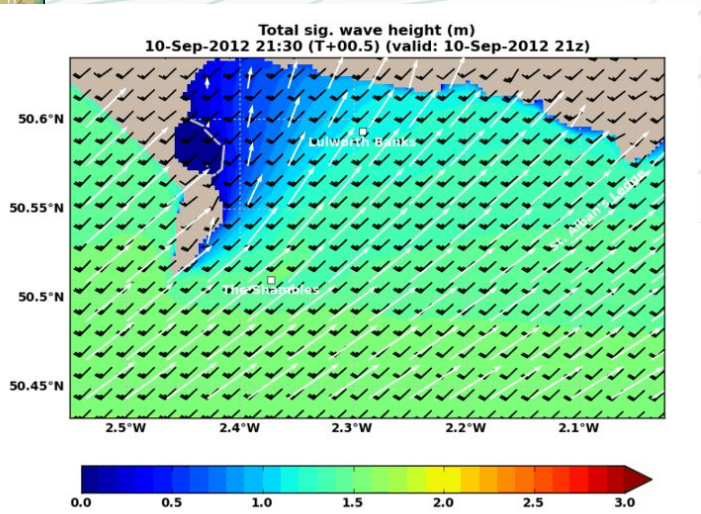
300 km



30 km



300 m



A factor of 1000 between these

…the same scheme has to continue to work

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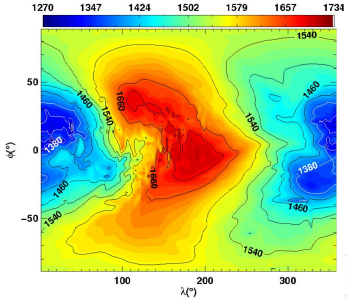
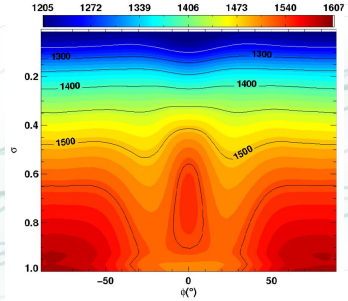
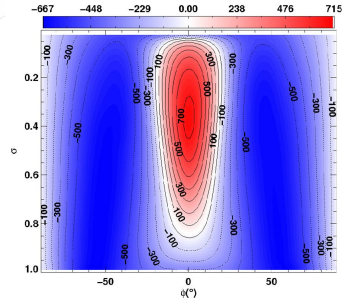
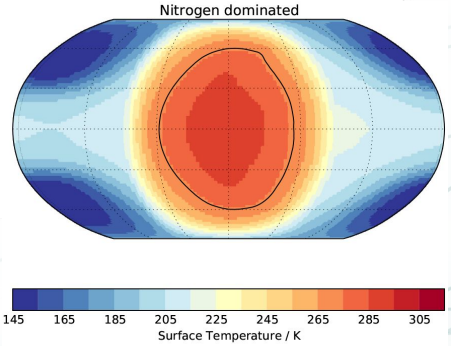
Exoplanets

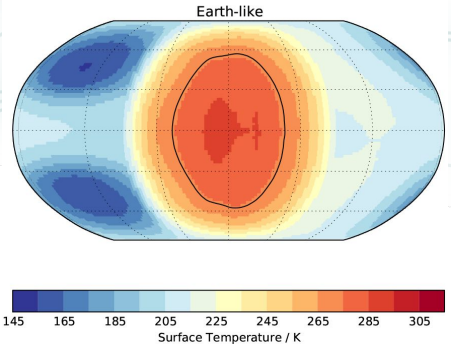
The unified model, a fully-compressible, non-hydrostatic, deep atmosphere global circulation model, applied to hot Jupiters
Mayne *et al.* 2014











Exploring the climate of Proxima B with the Met Office Unified Model
Boutle *et al.* 2017

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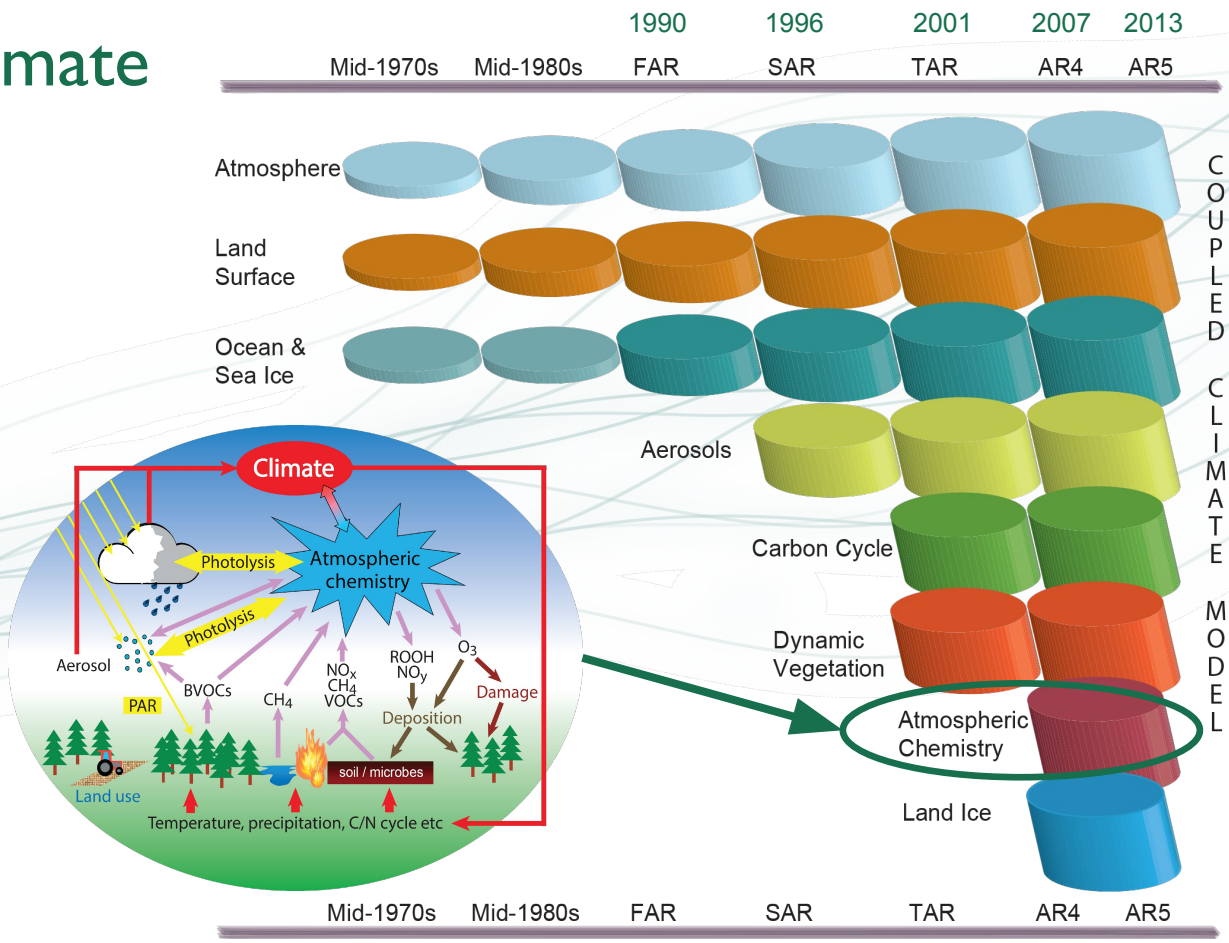
Development of Climate Models

Increasing the **number** and **complexity** of processes represented in climate models.



IPCC, 2013

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United Kingdom Chemistry and Aerosols

- In Cambridge we work on a part of the UM called the *United Kingdom Chemistry and Aerosols* sub-model, or **UKCA**.
- We develop new chemistry schemes for the model, with a focus on Chemistry-Climate Interactions.
- Here we usually include between 75-240 transported chemical species and hundreds of reactions to allow the model to accurately simulate changes to radiatively important gases such as ozone and methane, which can feed-back on the climate system.

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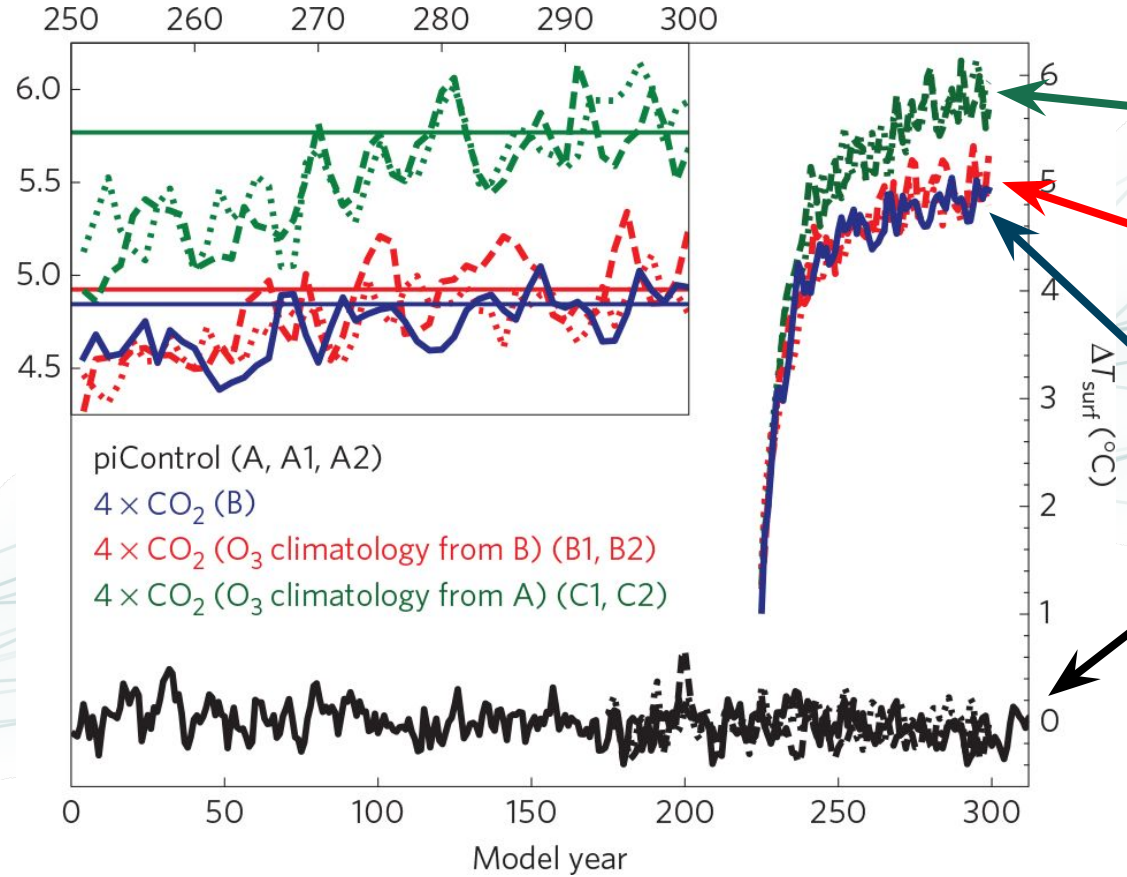
Chemistry-Climate Interactions



Prescribed pre-industrial ozone from A

Prescribed ozone from B

Interactive chemistry (B)

Pre-industrial control simulation (A)

Nowack *et al.*, *Nature Climate Change*, 2014

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4xCO2

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Developing code for the Unified Model

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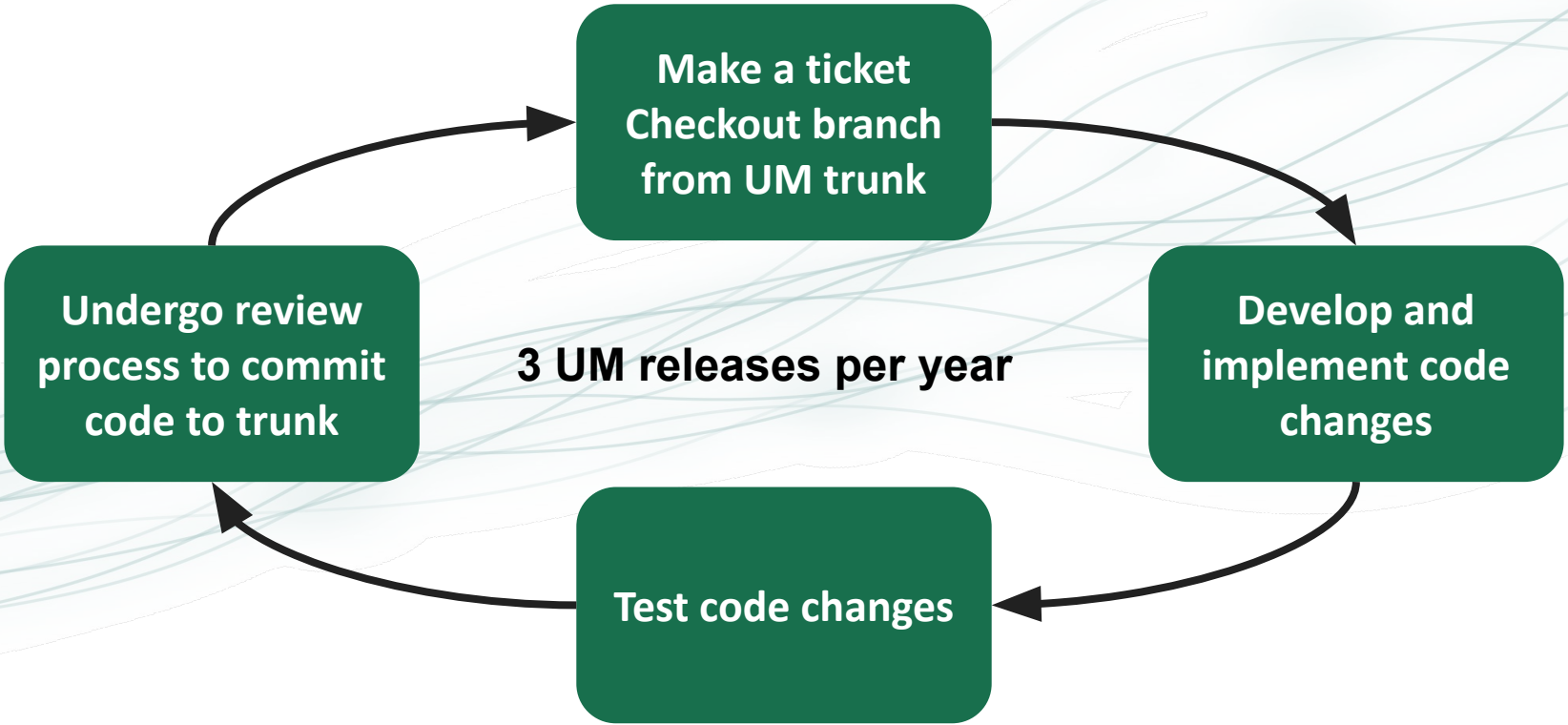
The Met Office Unified Model

um | Unified Model

- Approximately 900,000 lines of code (mainly Fortran 2003).
- Over 200 active developers.
- Uses the *Rose* graphical namelist editor and the *Cylc* workflow engine, with the code held in subversion repositories, managed using *FCM* ("Flexible Configuration Management" - mostly a wrapper around subversion).
- Majority of the development work is done by the Met Office.

Met Office Unified Model code development process



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Similar process for science improvements to be included in operational configurations.

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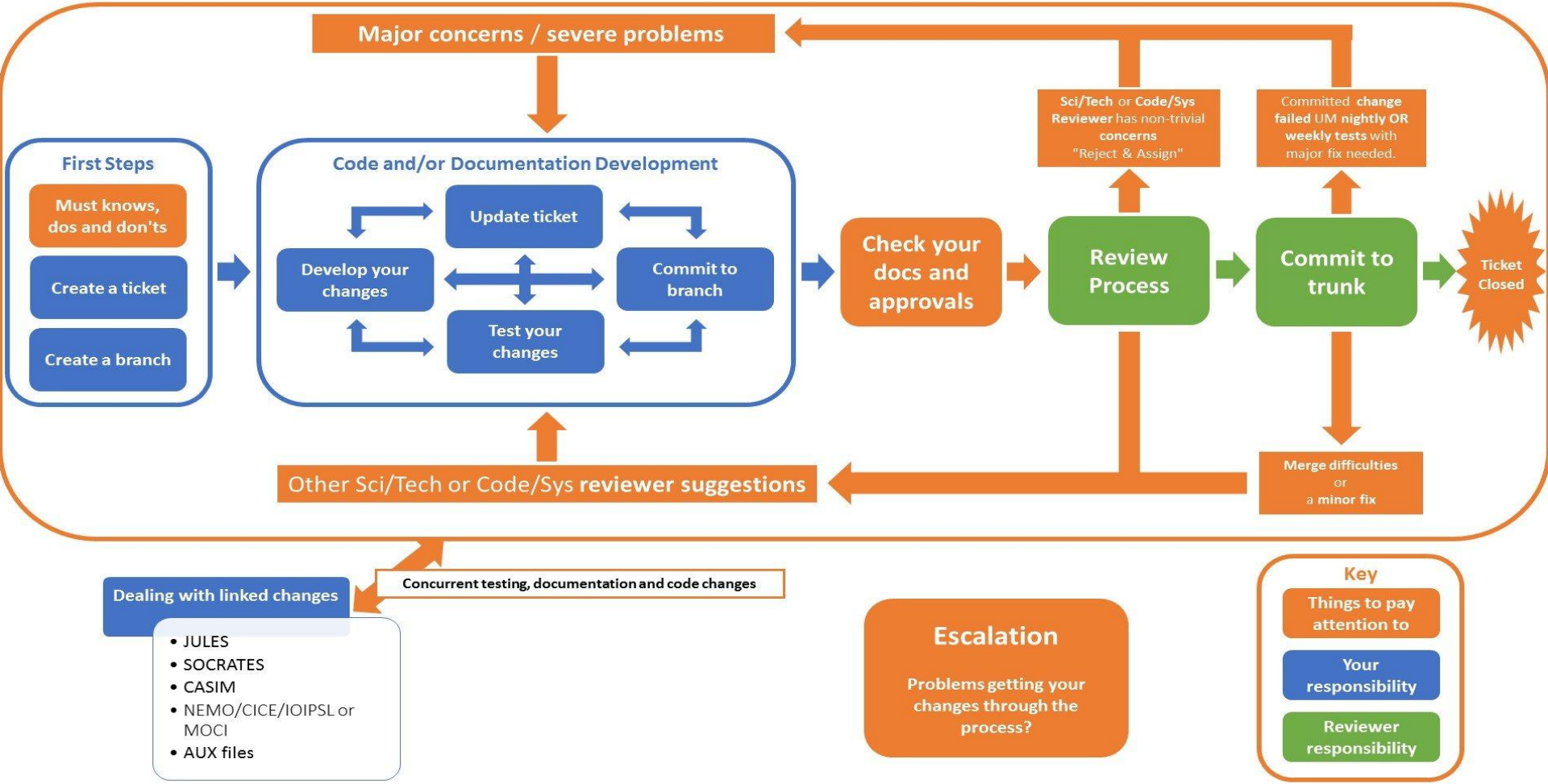
UM Development Working Practices



Code development process

- Science changes often require testing with long simulations that will take several weeks or more to run.
  - Diagnostics are then run through assessment and validation tools to produce many plots of standard metrics.

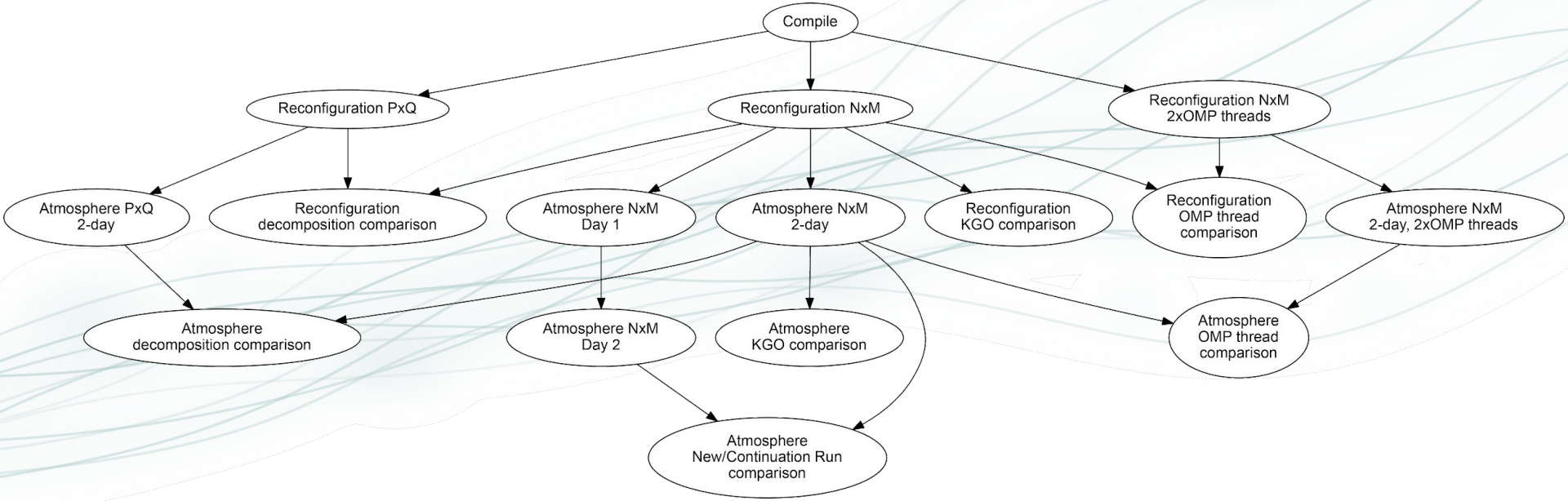
- All code changes are tested using the *rose-stem* utility, using a set of standard tests that compare against "***Known Good Output***" *(KGO).*
  - e.g. a climate resolution UKCA testing job takes 7 minutes to run 2 model days on 144 cores, requiring 112GB of memory.

- **You must be able to show that your change works when turned on and doesn't break anything when turned off.**

rose-stem

- At UM vn12.2 there are 328 UM testing jobs (inc. 33 UKCA jobs):
  - HPC jobs with Cray, GCC/Intel & GNU compilers
  - Linux jobs GCC/Intel, GCC/PGI, Clang/Intel, & GNU compilers
- Additional restart file creation tests and further tests for code standards, metadata, utilities, creation of boundary conditions, etc.
- Tests include KGO, restartability, OpenMP, & processor decomposition tests, with a range of optimisation levels:
  - “high”, “fast”, “safe”, “debug”, “rigorous”.
- If a KGO test “breaks” you need to explain why and get approval to change the saved output.
- **Tests protect your code and scientific configurations from being broken by another change.**

rose-stem - Met Office testing framework



Done with different levels of compiler optimisation.

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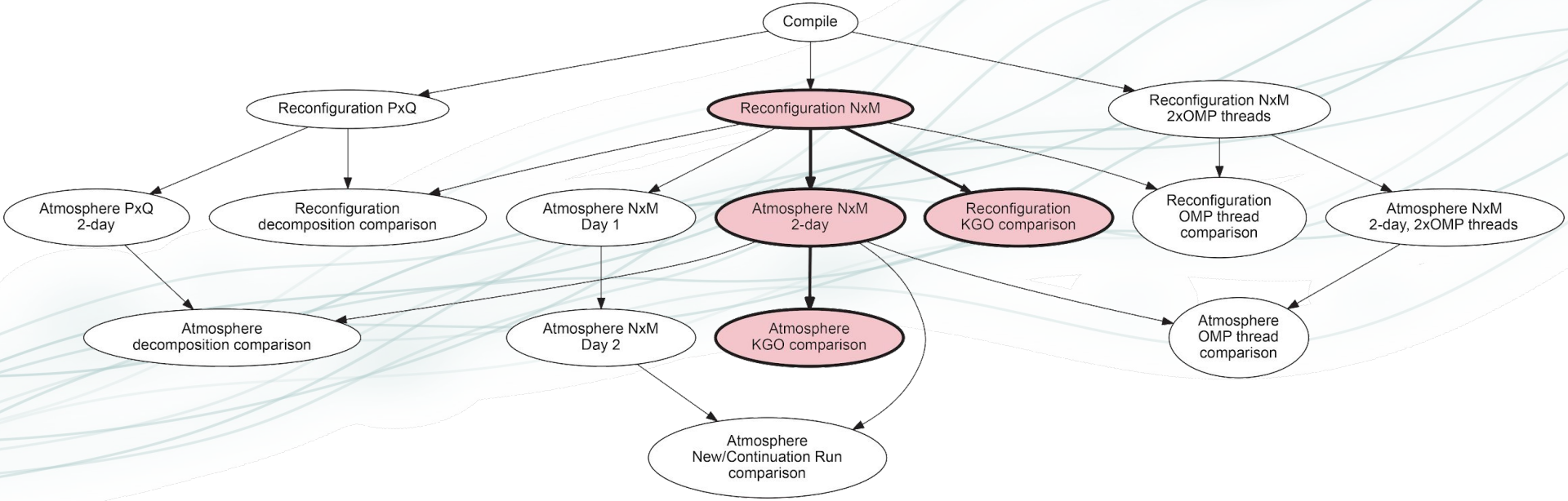
rose-stem - “Known Good Output” or KGO tests



KGO will likely be different with different levels of compiler optimisation.

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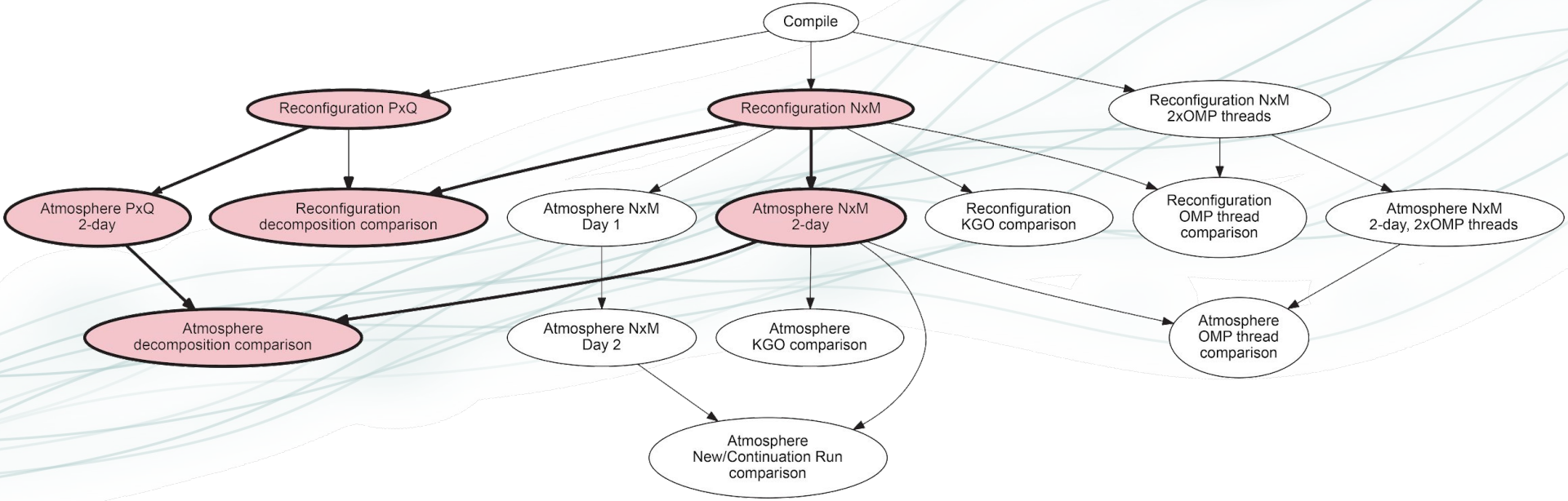
rose-stem - processor decomposition tests



Some changes may break KGO but should still pass the processor decomposition tests.

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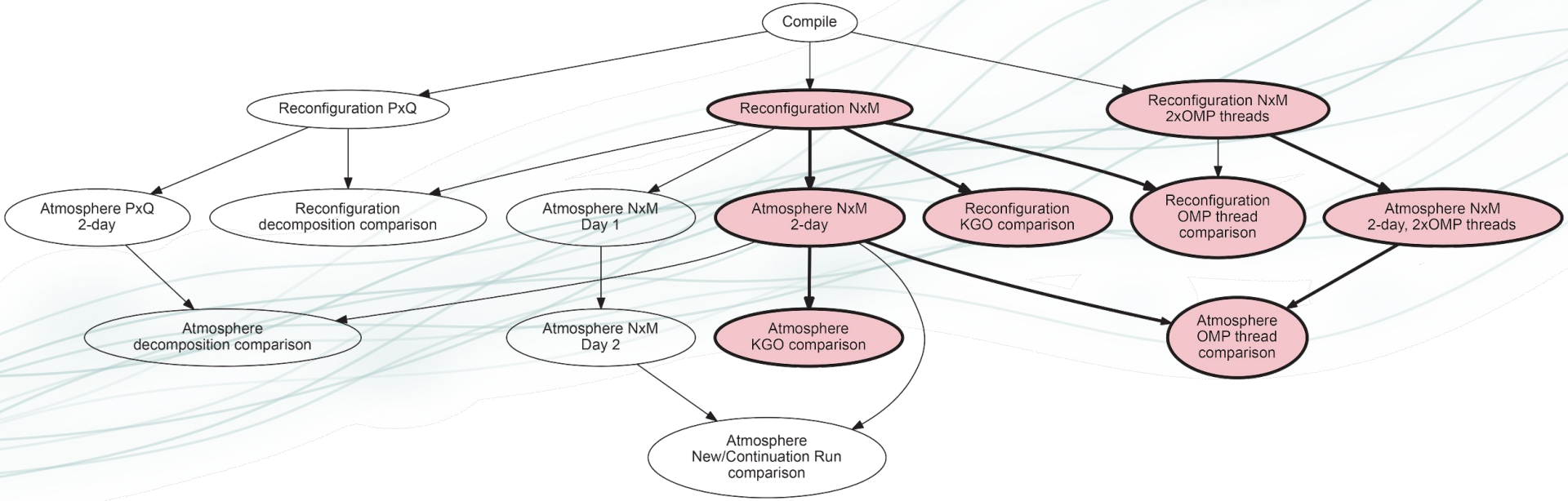
rose-stem - OpenMP tests



KGO should be identical with or without OpenMP, although the OMP test should still pass even if the KGO one does not.

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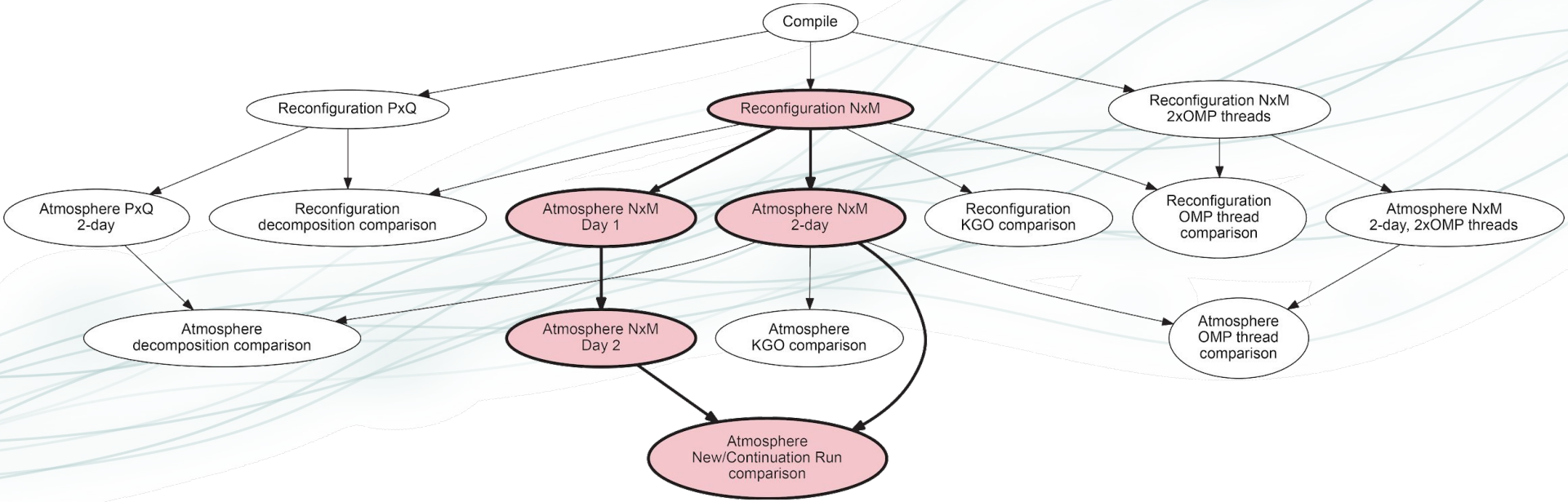
rose-stem - restart tests



Some changes may break KGO but should still pass the restartability tests.

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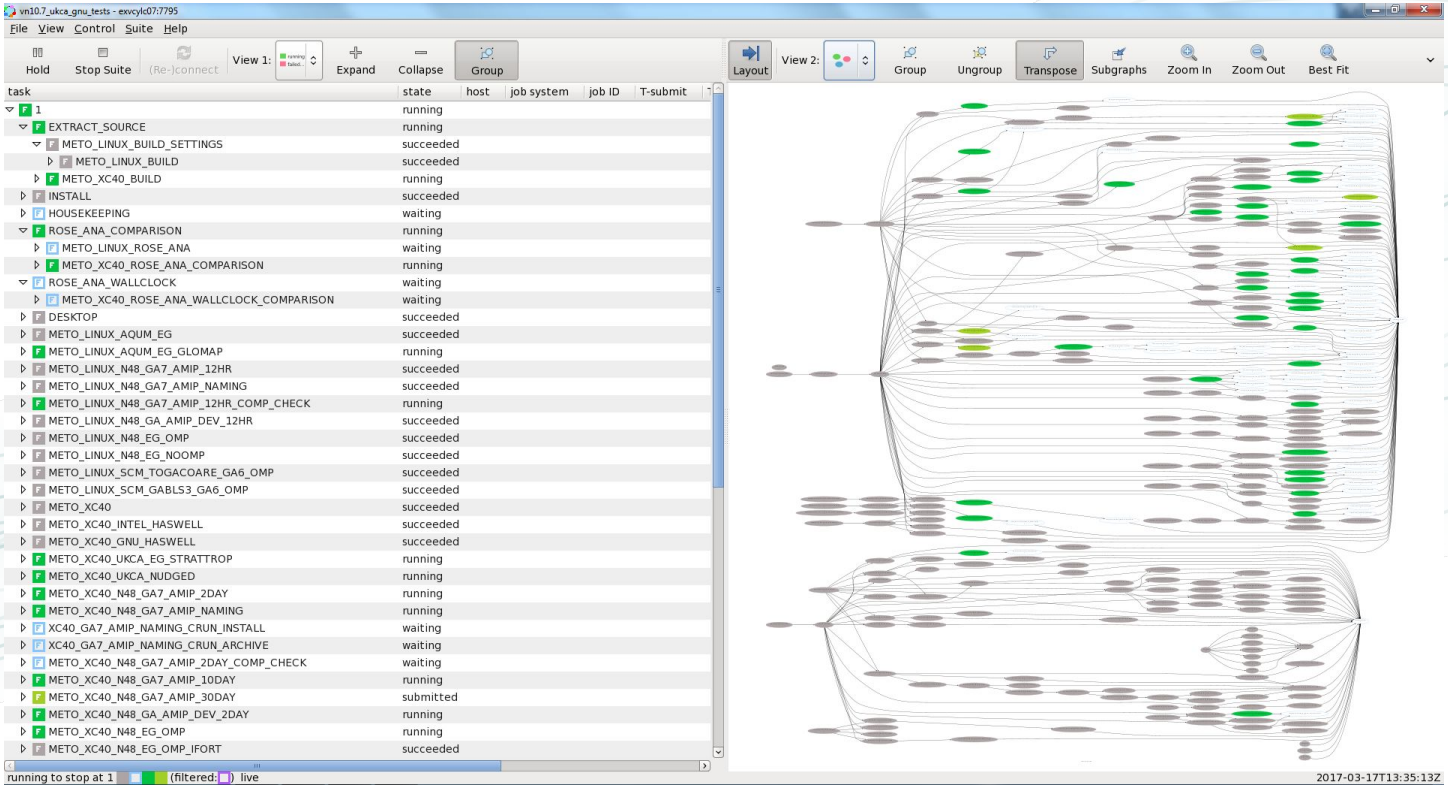
rose stem --group=developer,ukca



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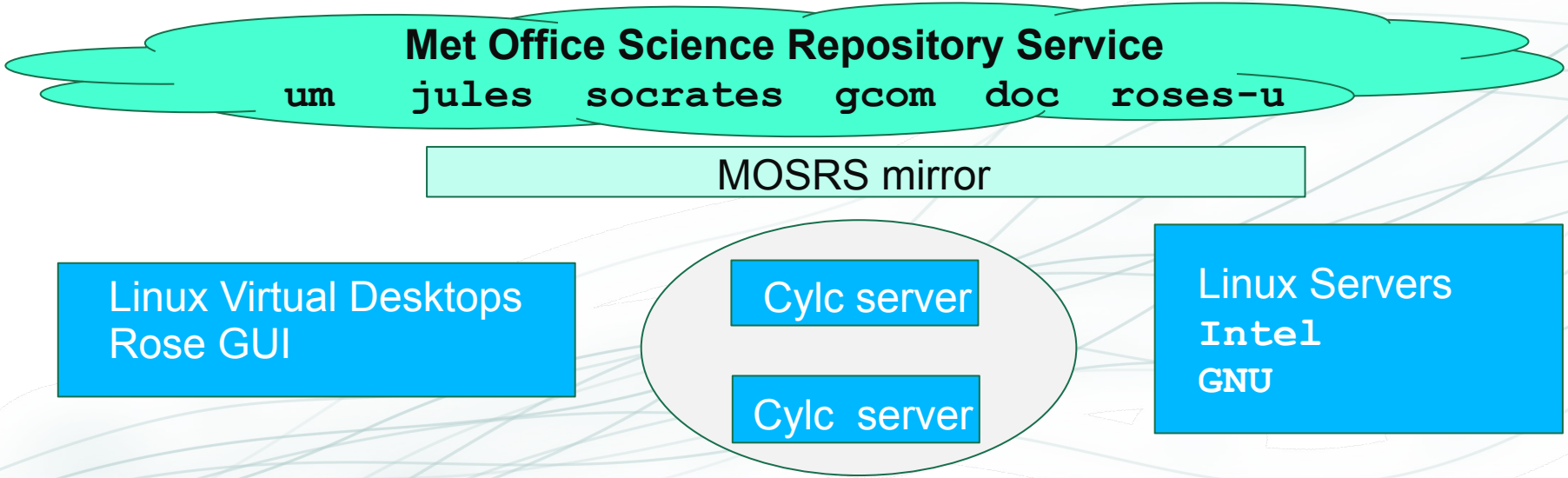
Met Office Infrastructure (2021)



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Outside the Met Office

But what if you don't have access to the Met Office infrastructure?

What can UK university students and researchers access?

- You should be able to get access to the UM source code and the tools to run the UM.
- You *may* be able to get access to HPC resources, e.g. ARCHER2 or Monsoon2 etc.
- You *may* be able to get access to an analysis platform, e.g. JASMIN.
- Access to rose-stem and the internal Met Office tools could be limited or not available at all.

What do I mean by "virtually"?

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What do I mean by *"virtually"*?

- A Virtual Machine configuration has been developed to allow people to easily use FCM, Rose, & Cylc.
- Uses Vagrant and VirtualBox (for a PC or server) or AWS.
- UM Systems Team have set-up running the UM in an Ubuntu guest image.

JASMIN

Met Office Virtual Machine on GitHub:

`https://github.com/metomi/metomi-vms`

aws

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Uses for the VM

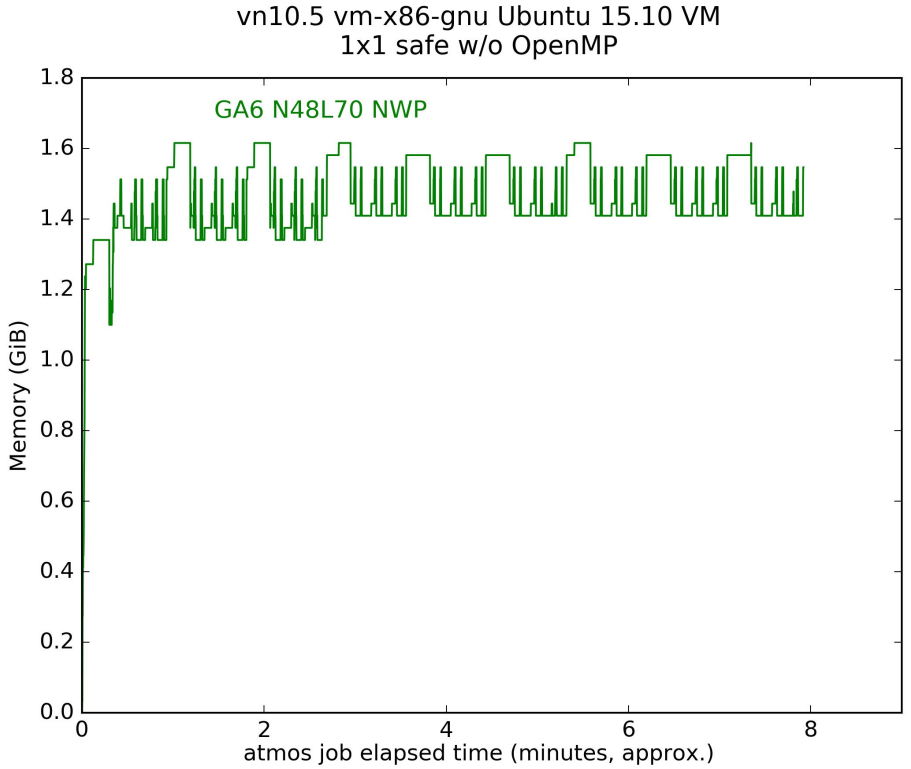
1. Developing & testing code changes
    - Faster turnaround time
        - Approximately 10 minutes to compile from scratch, with only a few seconds to recompile.
        - Small versions of standard jobs run in a few minutes on 2 cores.
2. Training

What do I mean by *"virtually"*?

- To run a basic UM test suite, the VM needs around 3GB of memory.
- Initial thoughts were that the main issue with running UKCA would (*probably!*) be the memory requirement.
  - A standard UKCA job requires an additional 137 3D fields to be added to the restart file, along with further temporary arrays allocated at run-time and any extra required for diagnostic output.
  - Usually require at least 112GB of memory at climate resolution (192x144x85 grid points).

Memory usage for um-atmos job

Basic test suite uses ~1.6GiB



GA6 job runs for 9 model hours
- 27 timesteps

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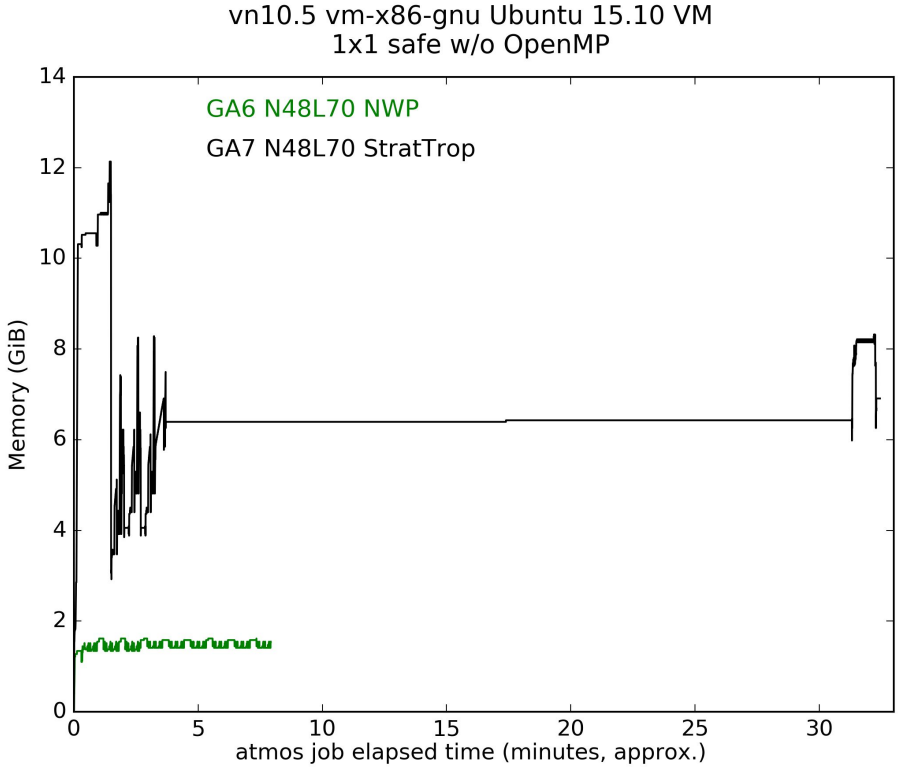
Memory usage for um-atmos job

Basic test suite uses ~1.6GiB

Low resolution UKCA suite uses ~12.2GiB



GA6 job runs for 9 model hours
- 27 timesteps
GA7 jobs run for 1 model hour
- 3 timesteps for L70

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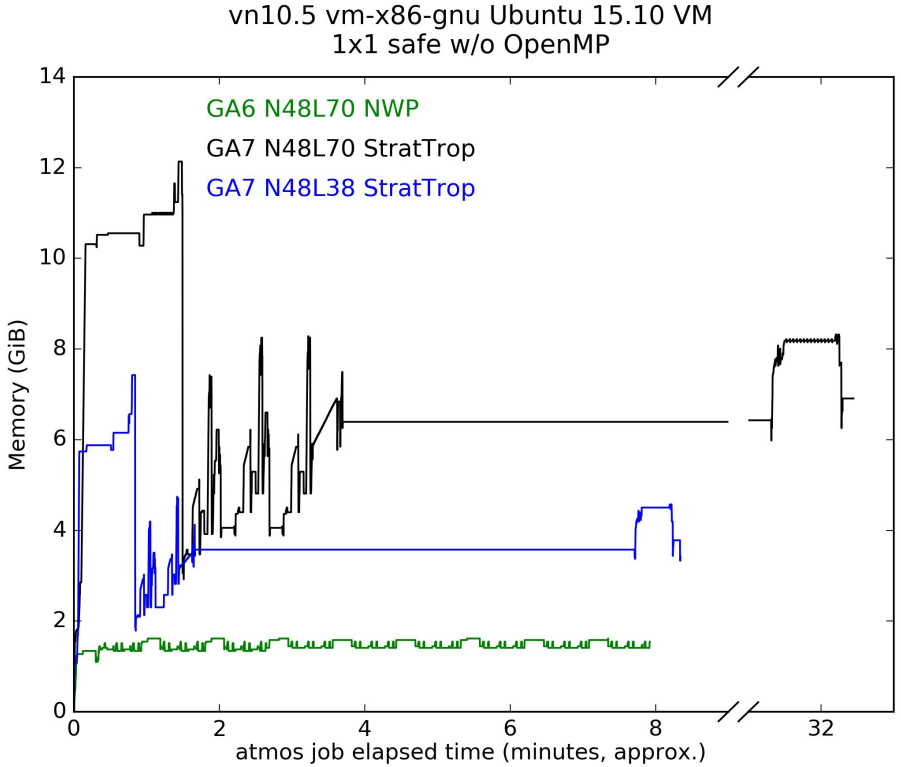
Memory usage for um-atmos job

Basic test suite uses ~1.6GiB

Low resolution UKCA suite uses ~12.2GiB

Low resolution UKCA suite (low top) uses ~7.4GiB



GA6 job runs for 9 model hours
- 27 timesteps
GA7 jobs run for 1 model hour
- 3 timesteps for L70
- 2 timesteps for L38

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Memory usage for um-atmos job

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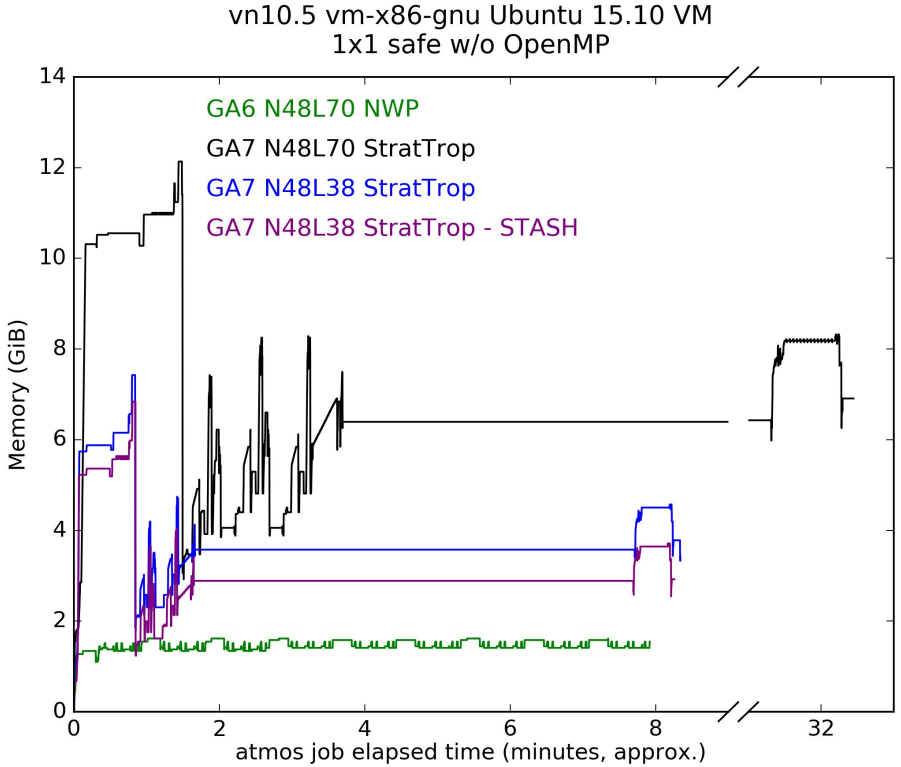
Low resolution UKCA suite (low top) uses ~6.9GiB when all diagnostic output requests are removed



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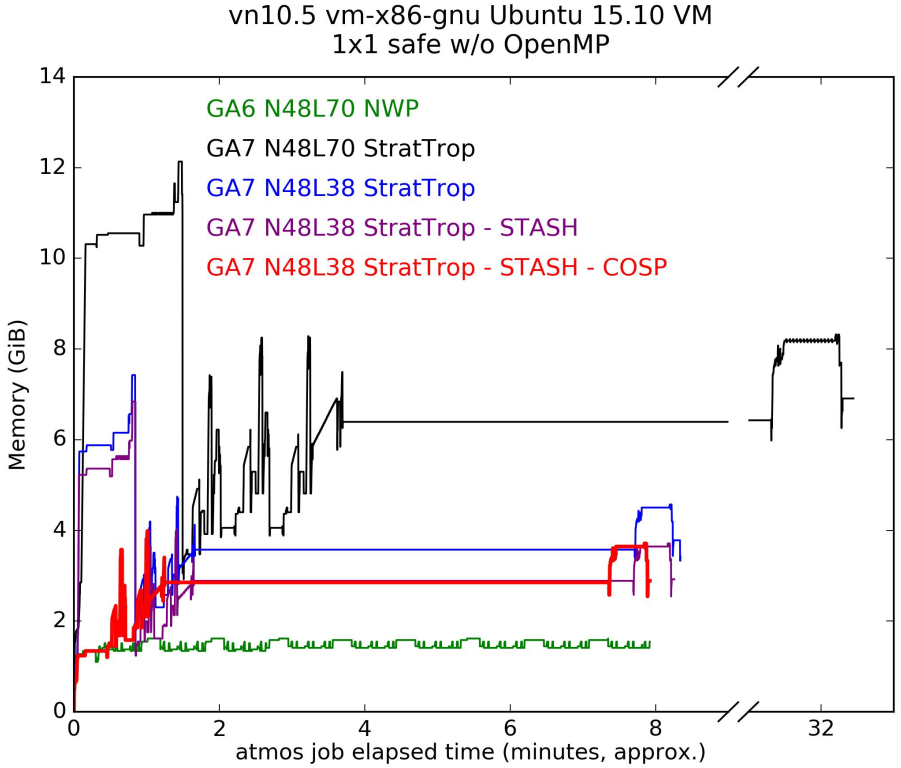
Low resolution UKCA suite (low top) uses ~7.4GiB

Low resolution UKCA suite (low top) uses ~6.9GiB when all diagnostic output requests are removed

Low resolution UKCA suite (low top) uses ~4.0GiB when all diagnostic output requests are removed and the COSP (*CFMIP Observation Simulator*) diagnostics package is not turned on



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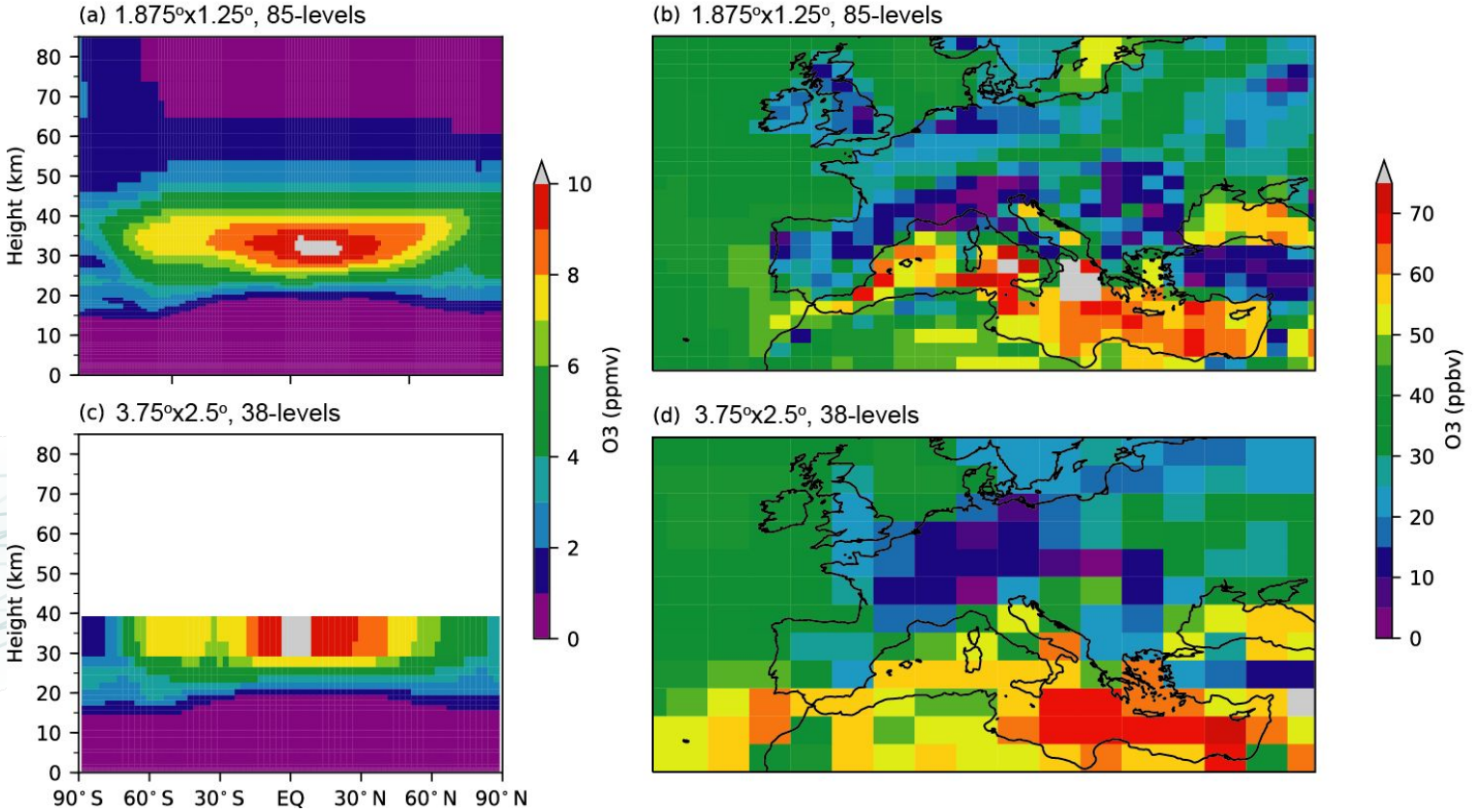
Climate resolution
192x144x85
grid points

VM-suitable resolution
96x72x38
grid points



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What do I mean by "virtually everything"?

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Helpful(?!) Errors

- However, there seemed to be an issue with using the GNU compiler, as the code failed with the following error on timestep 3:

```
?  Error from routine: EG_BICGSTAB_MIXED_PREC
?  Error message: NaNs in error term in BiCGstab
?        This is a common point for the model to fail if it
?        has ingested or developed NaNs or infinities
?        elsewhere in the code.
?        See the following URL for more information:
? https://code.metoffice.gov.uk/trac/um/wiki/KnownUMFailurePoints
```

- After some debugging, the issue *appeared* to be with the UKCA routine **`asad_hetero.F90`**, which couples the chemistry and aerosol schemes.

Precision

The UM uses compiler flags to make **`REAL`**s double-precision, so rather than using

```
REAL(KIND=8) :: a
```

or

```
INTEGER, PARAMETER :: dp=SELECTED_REAL_KIND(15,300)

REAL(KIND=dp) :: a
```

the UM will use

`-r8` (Intel), **`-s default64`** (Cray), **`-fdefault-real-8`** (GNU)

AND there is still the occasional **`1.0d0`** statement.

But what about `TINY(1.0d0)`?

- Intel (`-r8`):

```
tiny(1.0)    =   2.225073858507201E-308
tiny(1.0d0)  =   2.225073858507201E-308
```

- Cray (`-s default64`)

```
tiny(1.0)    =  2.22507385850720138E-308
tiny(1.0d0)  =  2.22507385850720138E-308
```

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- Cray (`-s default64`)

```
tiny(1.0)    =   2.22507385850720138E-308
tiny(1.0d0)  =   2.22507385850720138E-308
```

- GNU (`-fdefault-real-8`)

```
tiny(1.0)    =    2.2250738585072014E-308
tiny(1.0d0)  =    3.36210314311209350626267781732175260E-4932
```

Effectively `a = 1.0d0 = 1.0`

but `a = tiny(1.0d0) = 0.0`

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But what about `TINY(1.0d0)`?

- Intel (`-r8`):

```
tiny(1.0)    =    2.225073858507201E-308
tiny(1.0d0)  =    2.225073858507201E-308
```

- Cray (`-s default64`)

```
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tiny(1.0d0)  =   2.22507385850720138E-308
```

- GNU (`-fdefault-real-8`)

```
tiny(1.0)    =    2.2250738585072014E-308
tiny(1.0d0)  =    3.36210314311209350626267781732175260E-4932
```

- GNU (`-fdefault-real-8 -fdefault-double-8`)

```
tiny(1.0)    =    2.2250738585072014E-308
tiny(1.0d0)  =    2.2250738585072014E-308
```

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What do I mean by "everything"?

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Rose stem (again!)

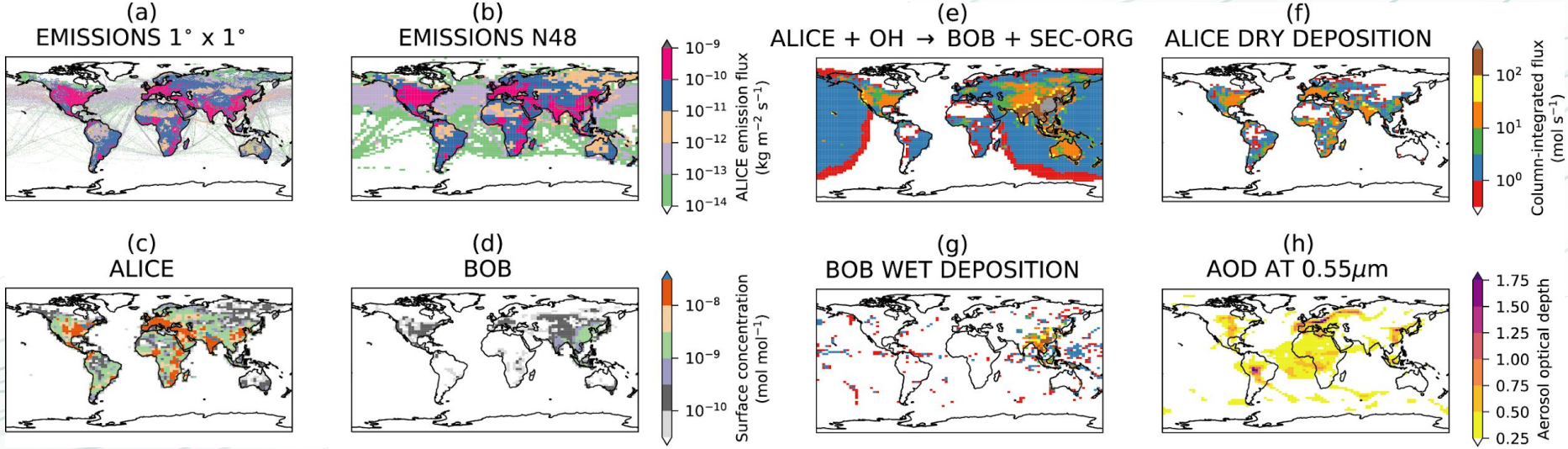
- These compiler flag changes went into the UM trunk at vn10.7.
- There are *rose-stem* testing jobs for several UM configurations (now also including UKCA) on the VM.
- Equivalent low-resolution UKCA jobs have also been added to the Met Office HPC tests.
    - One is included as part of the standard *developer* group that must be used when making any change.

Training

- What if we could use the VM for training?
- This would mean:

1. Everyone runs on their own dedicated computer.
    - Simpler set-up than for current production runs.
2. Researchers doing the tutorials can easily do the training tasks without needing a supercomputer account.
    - “Try before you buy”

UKCA Training



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Conclusions

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Conclusions

- Testing environments, as well as production environments, are required to be able to develop code changes in a timely manner.
- A Virtual Machine environment has been developed by the Met Office that easily allows users to install their own copy of the UM.
- Standard tests have also been implemented on this system that can be used when developing new code changes.
- This creates a standard system that all non-Met Office developers can use to quickly implement and test changes, prior to running on a HPC.

Geosci. Model Dev., 11, 3647–3657, 2018
https://doi.org/10.5194/gmd-11-3647-2018

Geoscientific Model Development
Open Access
EGU

Using a virtual machine environment for developing, testing, and training for the UM-UKCA composition-climate model, using Unified Model version 10.9 and above

Nathan Luke Abraham[1,2], Alexander T. Archibald[1,2], Paul Cresswell[3], Sam Cusworth[3], Mohit Dalvi[3], David Matthews[3], Steven Wardle[3], and Stuart Whitehouse[3]

[1]Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK
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Received: 8 May 2018 – Discussion started: 18 May 2018
Revised: 10 August 2018 – Accepted: 23 August 2018 – Published: 6 September 2018

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Step	ARCHER (XC30)	XCS-C (XC40)	Virtual Machine
Cray `cce` initial compile	34 minutes	15 minutes	-
Cray `cce` incremental compile	5-7 minutes	3 minutes	-
Intel `ifort` initial compile	19 minutes	9 minutes	-
Intel `ifort` incremental compile	6-7 minutes	1 minute	-
GNU `gfortran` initial compile	-	4 minutes	8-10 minutes
GNU `gfortran` incremental compile	-	2-3 minutes	45 seconds
Reconfiguration task, used to produce the initial conditions file.	3-4 minutes (Intel, 6×4)	15-30 seconds (GNU, 4×9)	25-30 seconds (GNU, 1×2)
Atmosphere task	40 seconds (Intel, 6×4)	45 seconds (GNU, 4×9)	12 minutes (GNU, 1×2)

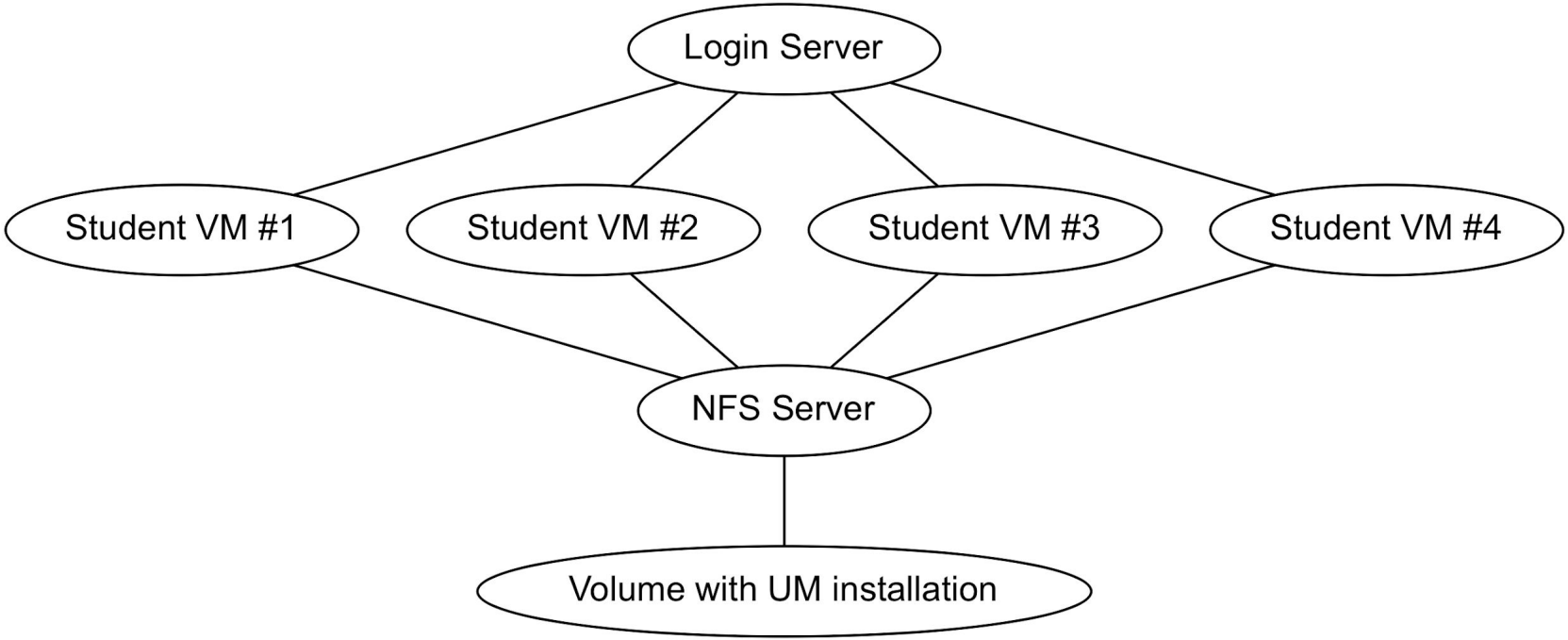
Compiler settings	**Safe**	**Safe**	**Rigorous**
Number of UM OpenMP threads	**0**	**2**	**2**
Approximate run-time on 2-core VM (1×2) (minutes)	8	11	29
Approximate run-time on 4-core VM (1×2) (minutes)	8	4	17
Approximate run-time on 4-core VM (1×4) (minutes)	5	8	22
Approximate run-time on 8-core VM (1×4) (minutes)	5	3	14
Approximate run-time on 8-core VM (1×8) (minutes)	3	6	26
Approximate run-time on 16-core VM (1×8) (minutes)	3	3	22

Compile type	GNU `gfortran` compiler flags	Number of UM OpenMP threads	Total VM memory required (GB)
safe	`-O2 -Werror`	0	6
safe	`-O2 -Werror` `-fopenmp`	2	6

rigorous	`-O0 -Wall`
	`-ffpe-trap=invalid,zero`
	`-fbounds-check`
	`-Warray-bounds`
	`-fcheck-array-temporaries`
	`-finit-real=nan`
	`-fimplicit-none`
	`-fopenmp`
		2	8

Training VMs on JASMIN

JASMIN



Ansible playbooks for this system are available via GitHub:
`https://github.com/theabro/ukca-playbook`

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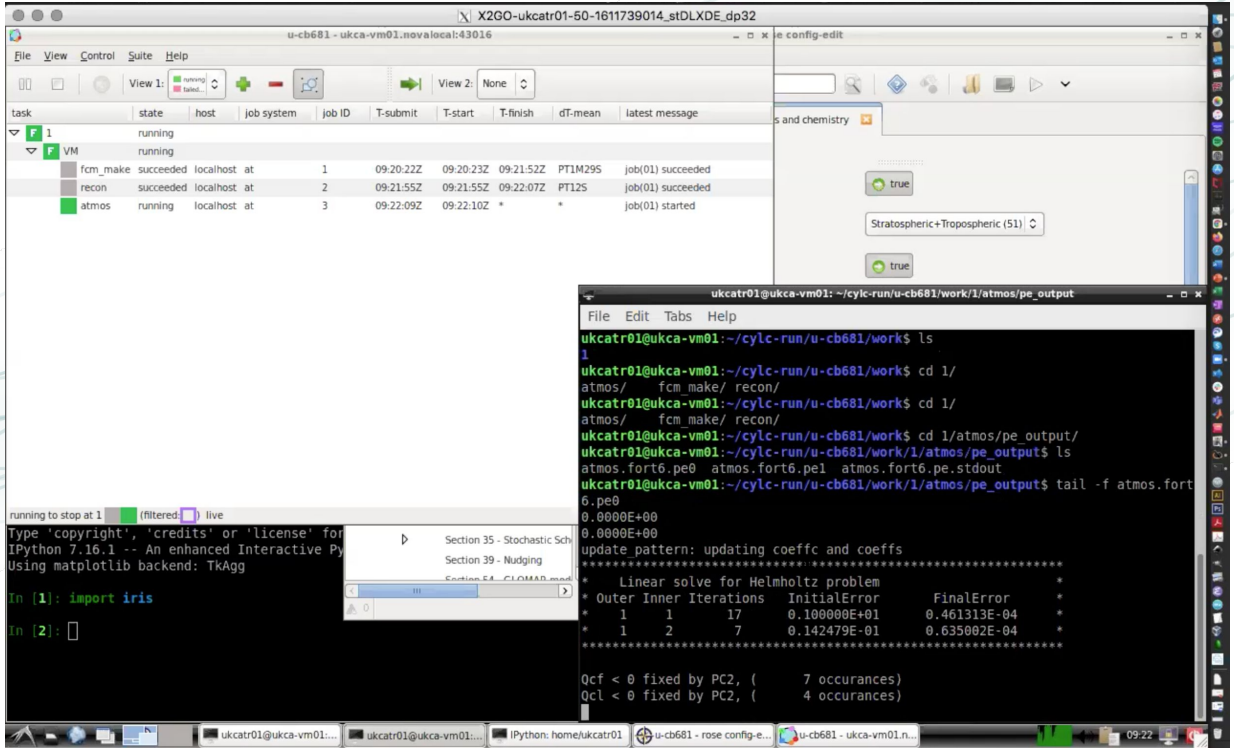
Training VMs on JASMIN

JASMIN

https://www.youtube.com/watch?v=5V3RBCYTQvg

Students could connect to their VM using a number of methods -
e.g. X2Go, MobaXTerm, or Terminal/X11

Set-up video with demonstration available on the UKCA YouTube channel.



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