



UNIVERSITY OF  
CAMBRIDGE

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Chemistry

# UKCA Training January/February 2024



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# Welcome

Welcome to the NCAS Introduction to UKCA training event!

Due to the online delivery of the UKCA training, it is important that you continue to work through the UKCA Tutorials in your own time outside of the scheduled Zoom sessions.

The **#support** channel in the **ukca-training-2024** Slack workspace should be used to ask questions outside of the Zoom times.



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# Schedule

The Zoom sessions will be each day

- 10am-11am: presentation(s) via Zoom
- 11am-12noon: debugging & technical support via Zoom
- 1pm-2.30pm: debugging & technical support via Zoom
- 9am-5pm: debugging & technical support via Slack workspace

The Zoom presentations (except Tuesday) will be recorded - please turn off your camera and mute yourself if you don't want to be seen.

**Tuesday - please prepare a 5-10 minute talk** and send me the slides by the end of today please.



# Problems

You've decided (or been told) to use UKCA, but if you are the only person at your institution using it it can be difficult to get up and running.

It can also be very difficult to overcome and solve model problems.

- The UKCA tutorials have been developed to solve this first problem
- The second issue is addressed by the NCAS Computational Modelling Services (CMS) team based in Reading

<http://cms.ncas.ac.uk/>



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## Pptransfer ARCHER2 archive directory: “No such file or directory” error


 Unified Model  ARCHER2  PPTransfer



Luke 

2  Jan '23

Hello,

I have copied GA8 UM13.0 suite u-cq166 ([GA8.0/GC4.0 Standard Suites](#)) as u-ct789 and followed the necessary steps to allow for JASMIN pptransfer ([Configuring PPTransfer](#) ). This suite is running without issues and archives the data to JASMIN.

I have then copied this suite and added the necessary UKCA changes (mainly to app/um). The original suite for this is u-cq018 which runs on Monsoon2 ([GA7.1 StratTrop suites - UKCA](#)).

This suite also runs, but is failing on the pptransfer task with the error

```
[WARN] [SUBPROCESS]: Command: ls -A /work/n02/n02/luke/archive/u-ct792/19880901T0000Z  
[SUBPROCESS]: Error = 2:  
ls: cannot access '/work/n02/n02/luke/archive/u-ct792/19880901T0000Z': No such file or directory
```

I'm wondering what I could have done differently between these jobs to cause this directory not to exist. I have noticed that the original GA8 job uses climate meaning whereas the UKCA version does not, instead having the postproc task produce these. The postproc version on Monsoon2 is 2.4 but it is 2.3 on ARCHER2. However, subsequently altering the postproc app to produce climate means doesn't seem to have done anything (but this was on running a second time after the postproc settings were updated).

I should add that there are quite a few changes to STASH in the UKCA job.

Are there any suggestions as to what might be going wrong here and how to fix it?



Jan 2023

1 / 4

Jan 2023

The Helpdesk is searchable, so if you have a problem the first thing to do is to search for past tickets with the same problem.

If you cannot find a solution open a new ticket. This will be emailed round to all of the CMS team.

Jan 2023



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# What is UKCA?

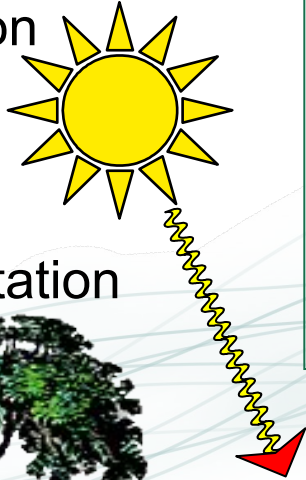


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# Atmospheric Modelling: integrating our knowledge of atmospheric behaviour forward in time

short-wave  
radiation



**Newton's laws  
for rotating fluid**

**Gas laws**

**Laws of  
thermodynamics**

vegetation

clouds



long-wave  
radiation

convection



precipitation

## Surface Processes

- 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

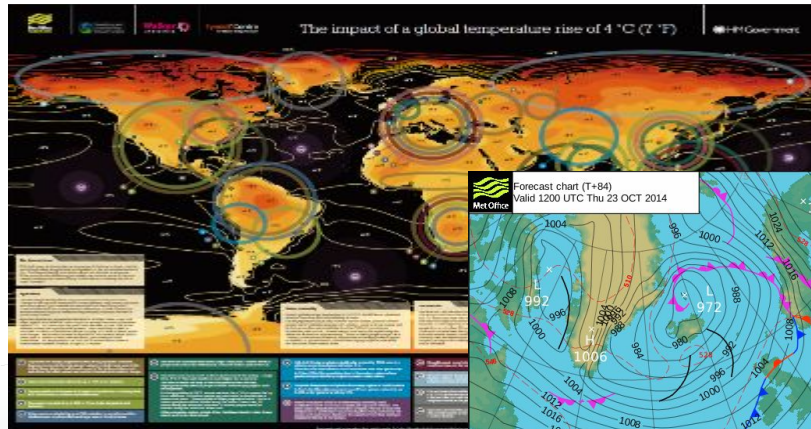
- Resolution 1km - 10m

> 25 years old

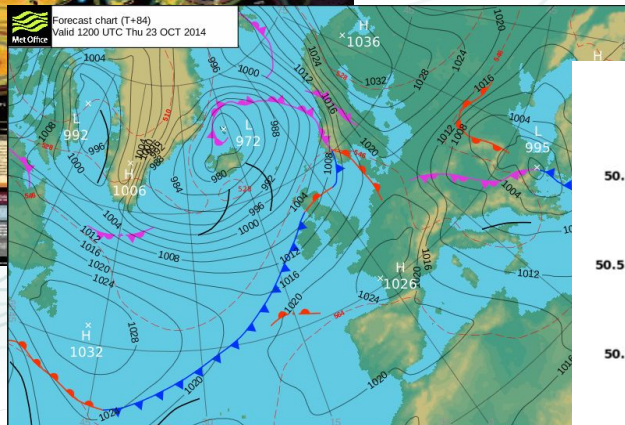


# The consequence of unification

300 km

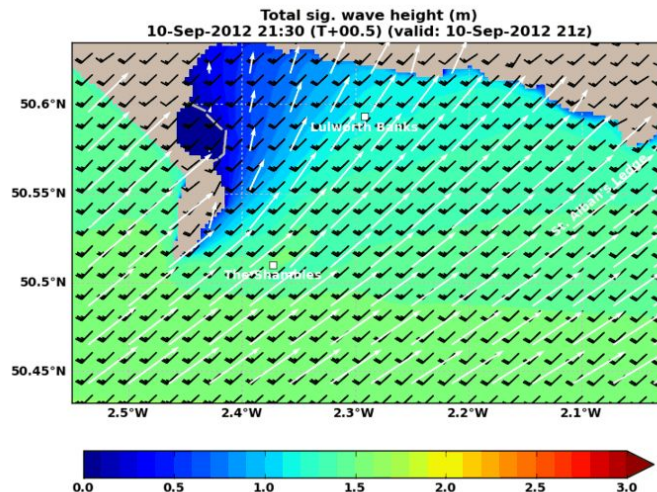


30 km



A factor of 1000  
between these

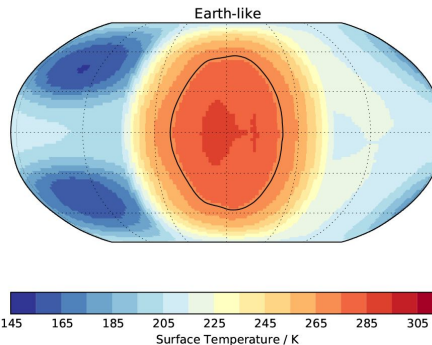
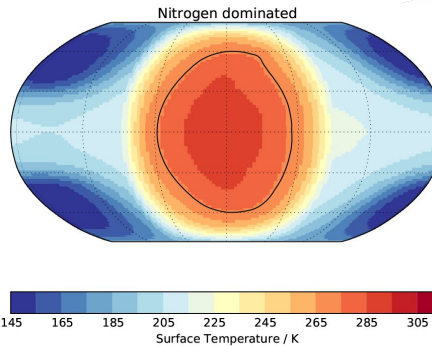
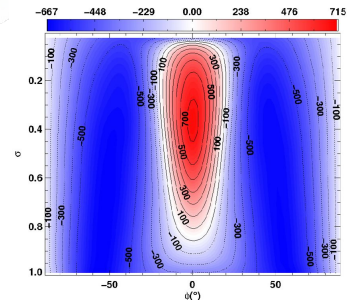
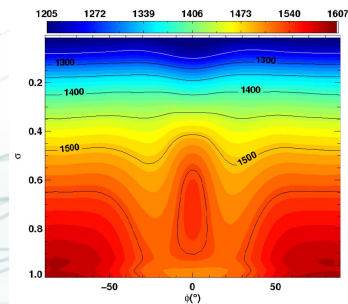
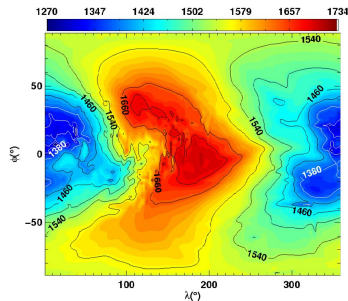
300 m



...the same scheme has  
to continue to work

# Exoplanets

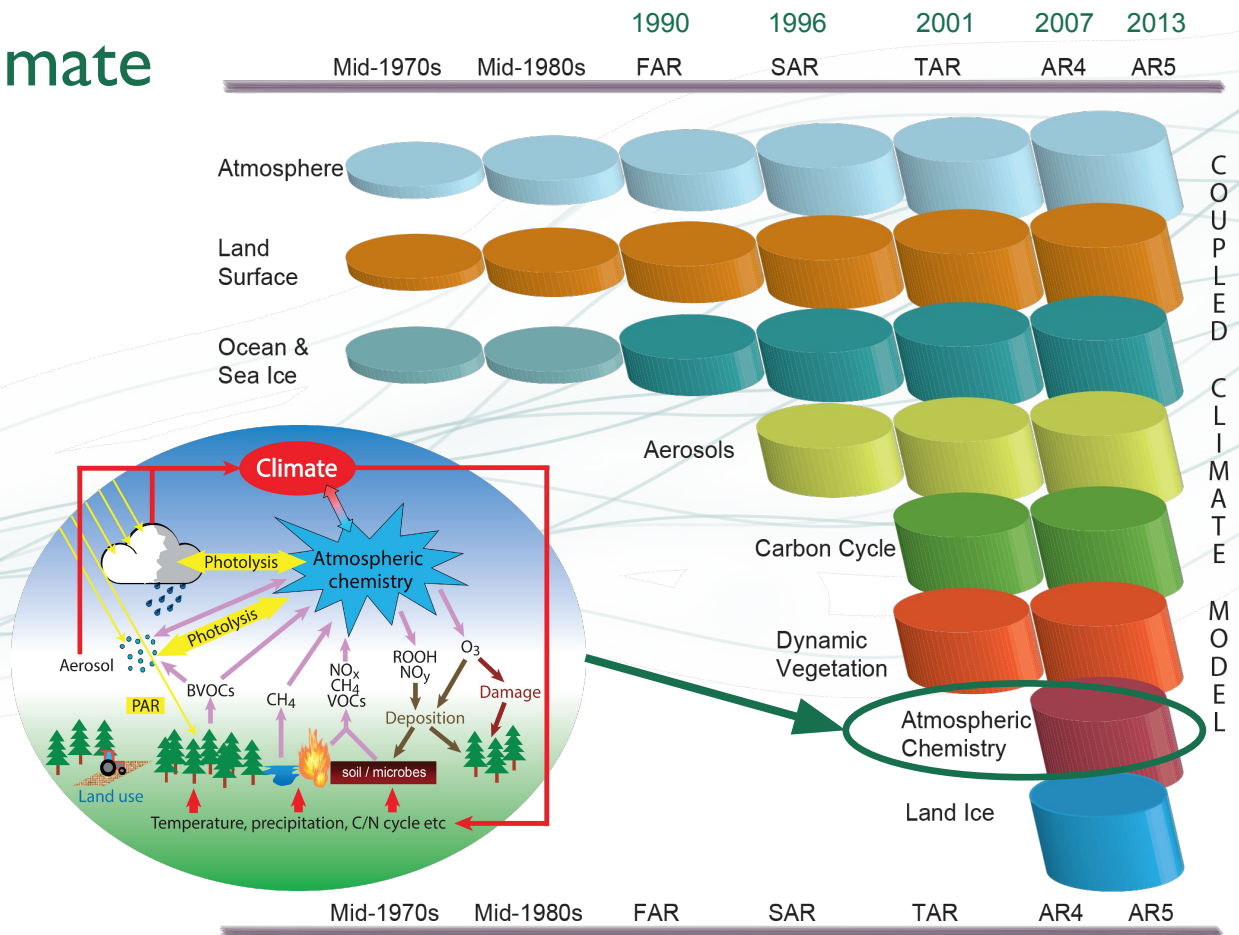
The unified model, a fully-compressible, non-hydrostatic, deep atmosphere global circulation model, applied to hot Jupiters  
Mayne *et al.* 2014



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

# Development of Climate Models

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

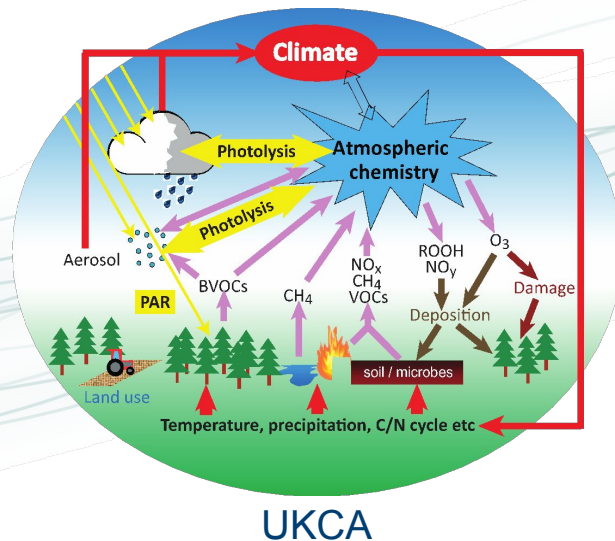


IPCC, 2013



# What is UKCA?

The **United Kingdom Chemistry and Aerosols** Model is not a *particular* collection of chemistry and aerosol schemes, but was designed to be a **framework** for putting chemistry and aerosol schemes into the Met Office Unified Model.

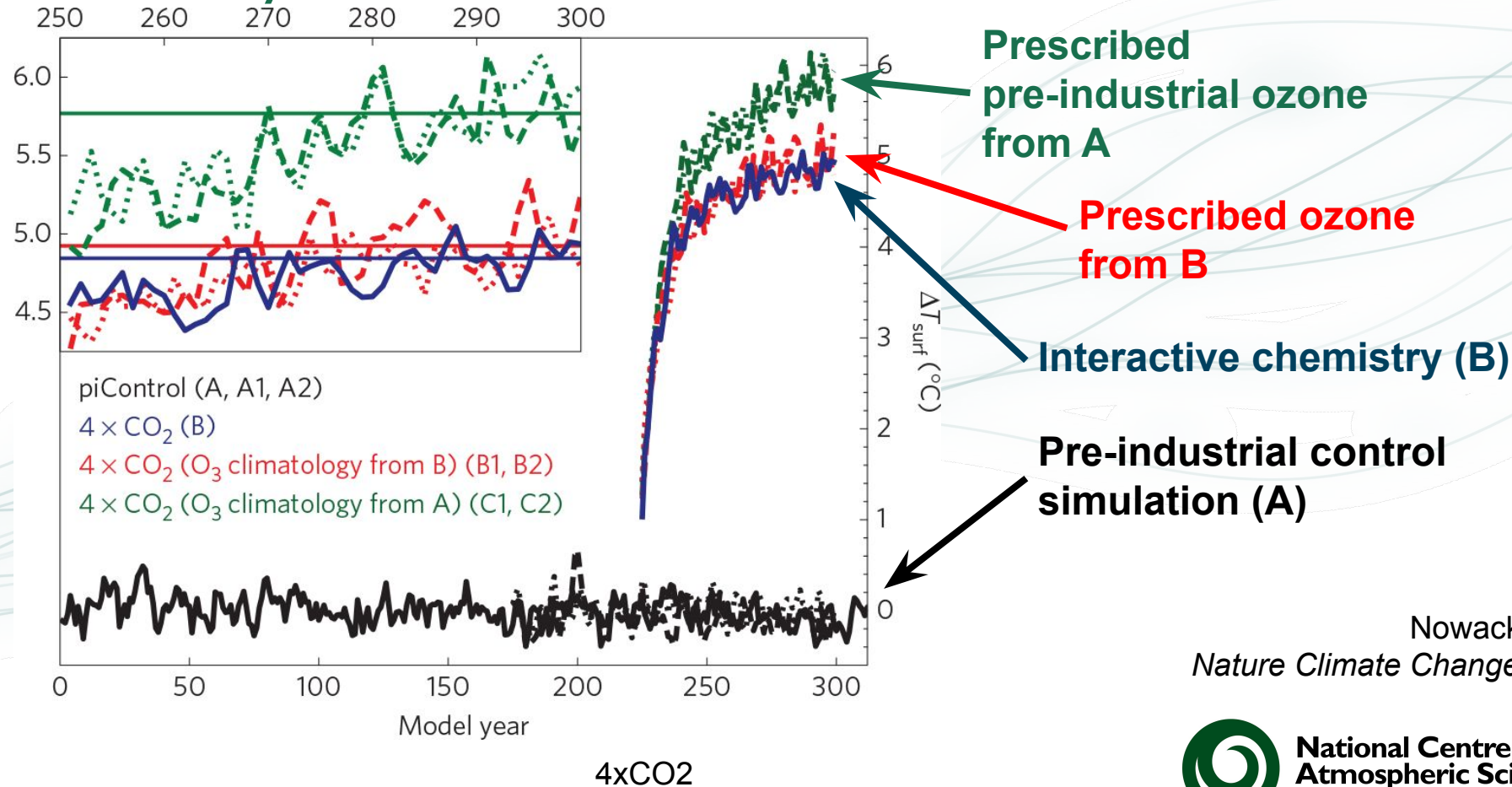


Unified Model



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# Chemistry-Climate Interactions



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

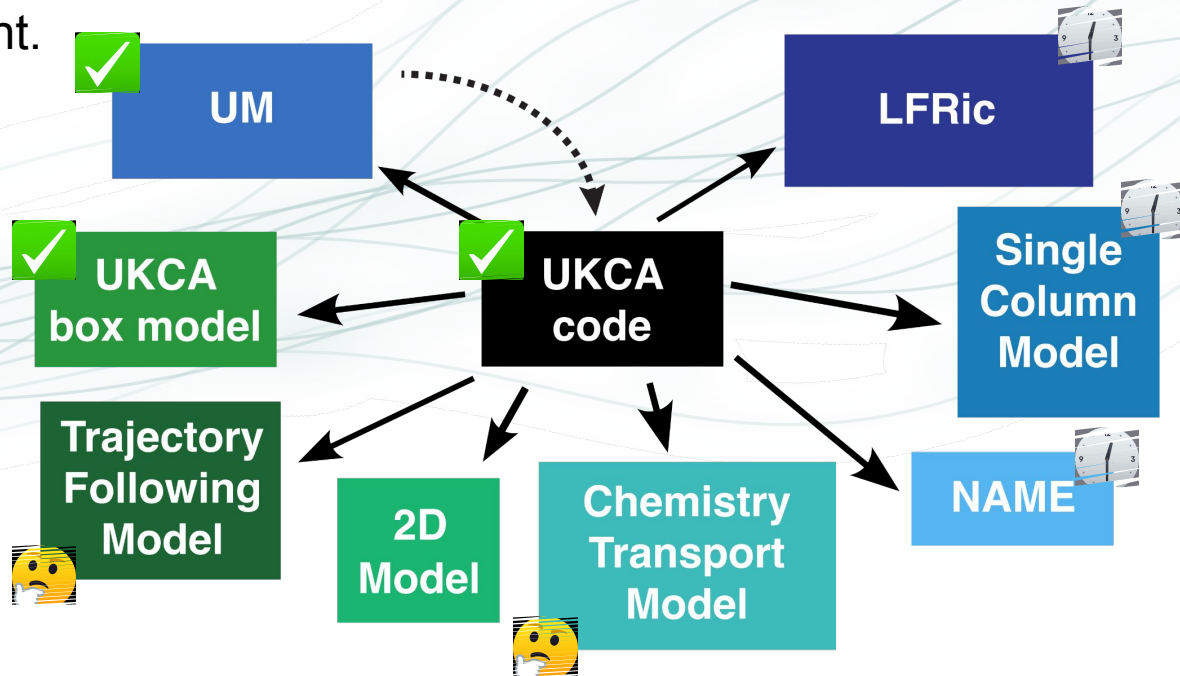
# UKCA Box Model

Recently we have developed a UKCA box model that allows for the running of UKCA at a single point.

Initial chemical, aerosol, and atmospheric conditions are specified by input files, and photolysis rates are currently specified in the same way.

The underlying UKCA routines have not changed.

This is designed to facilitate the coupling of UKCA to other parent models.





# UKCA repository

The work to make the UKCA box model also meant that we created a new UKCA repository on MOSRS. The UKCA code now exists there under an open-source BSD-3 license.

A directory structure has been imposed to the UKCA routines (over 140,000 lines of code across 258 files) to make things more organised.

<https://code.metoffice.gov.uk/trac/ukca/>



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wiki: [WikiStart](#) | [Start page](#) | [Index](#) | [History](#)

## Welcome to the United Kingdom Chemistry and Aerosols Project

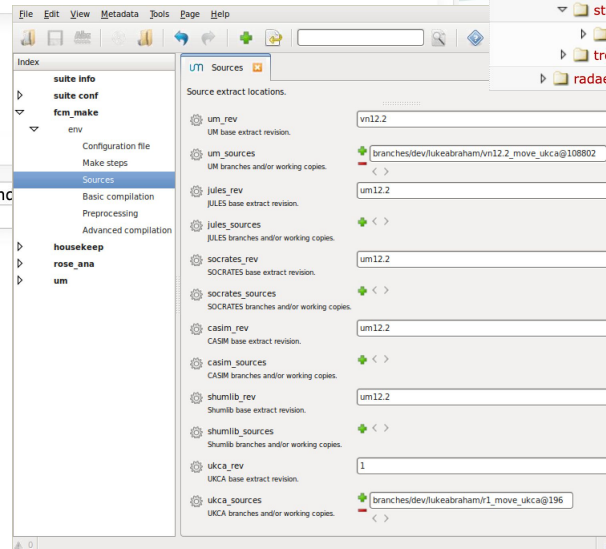
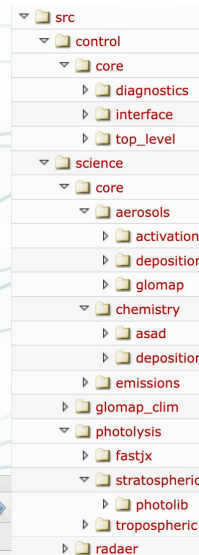
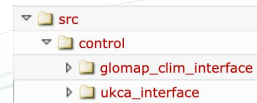
UKCA is a joint NCAS-Met Office programme part of the NERC-Met Office Joint Climate and Weather Research Programme (JWCRP). Project partners are the Hadley Centre and the Universities of Cambridge, Leeds and Oxford. Our objective is to develop, evaluate and make available a UK community atmospheric chemistry-aerosol model suitable for a range of topics in climate and environmental change research.

### Getting Started

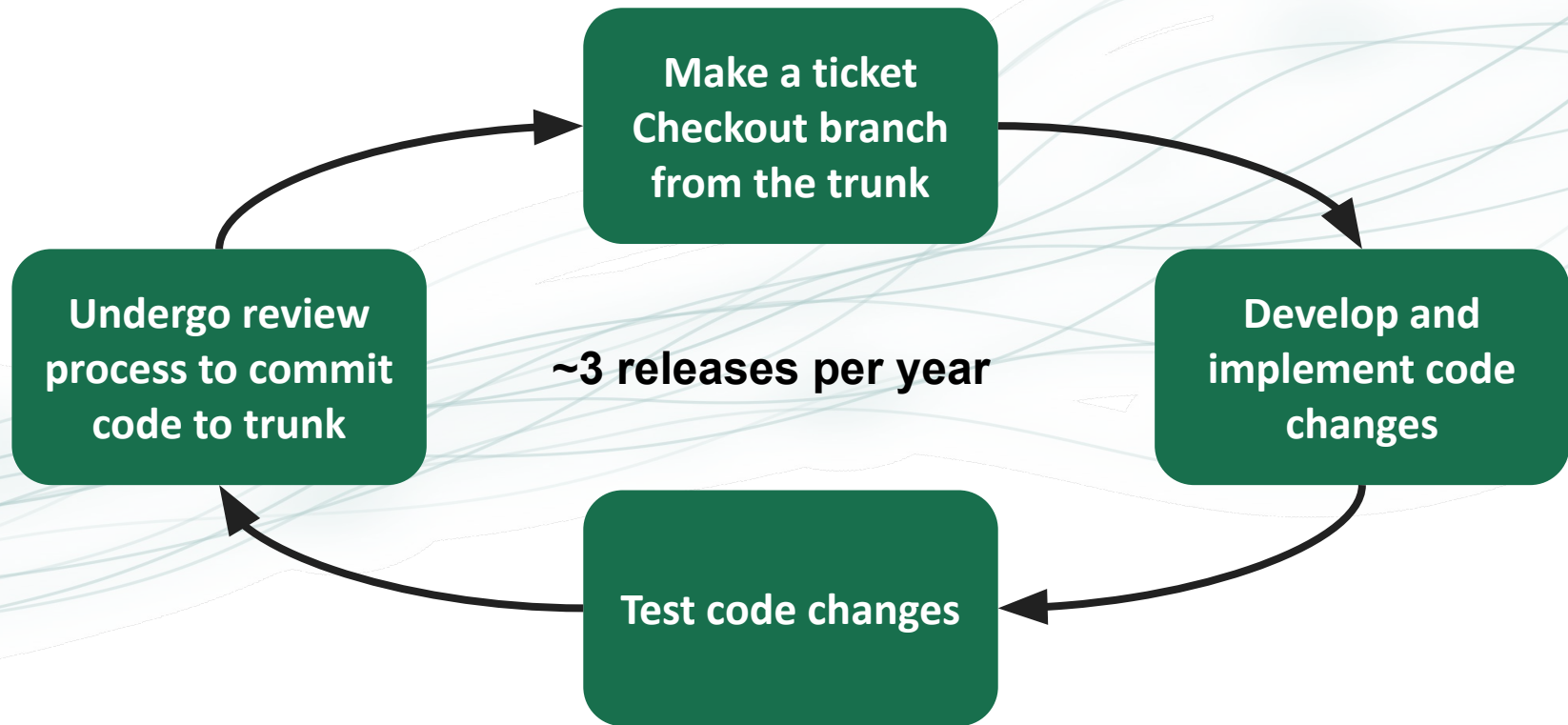
- [Working Practices](#)
- [UKCA License information](#)
- [UKCA Contributor License Agreement](#)
- [Meetings Page](#)

### Parent models

- |                               |                             |
|-------------------------------|-----------------------------|
| <a href="#">Unified Model</a> | Used as part of GA, GC, and |
| <a href="#">LFRic</a>         | Under development           |



# Met Office code development process



# Course Context

The training has been designed to teach new users of UKCA how to do a wide range of things with the current configuration that is used within the UK Earth System Model, but also covers more general points such as adding tracers, emissions, and UM output. The UKCA website has introductory videos on various aspects of UKCA, and there is a walkthrough provided for the tutorials.

Some parts will be easier than others, but don't worry if you have problems. Make use of the Slack channel to ask questions and also during the Zoom sessions.



# What can I do with UKCA?

- UKCA was originally designed to run for long integrations covering decadal to centennial timescales, but it can also be used for air-quality forecasts
- A number of different chemistry schemes currently exist in the model, which have been provided because the UKCA developers have wanted to use them for a particular purpose. If they don't suit your needs, then you can add to or change them
- One aim of the UKCA Tutorials is to teach you how to do this



*Premise:*

**What are the most common things that a PhD student or Research Associate will need to know how to do when they start using UKCA?**



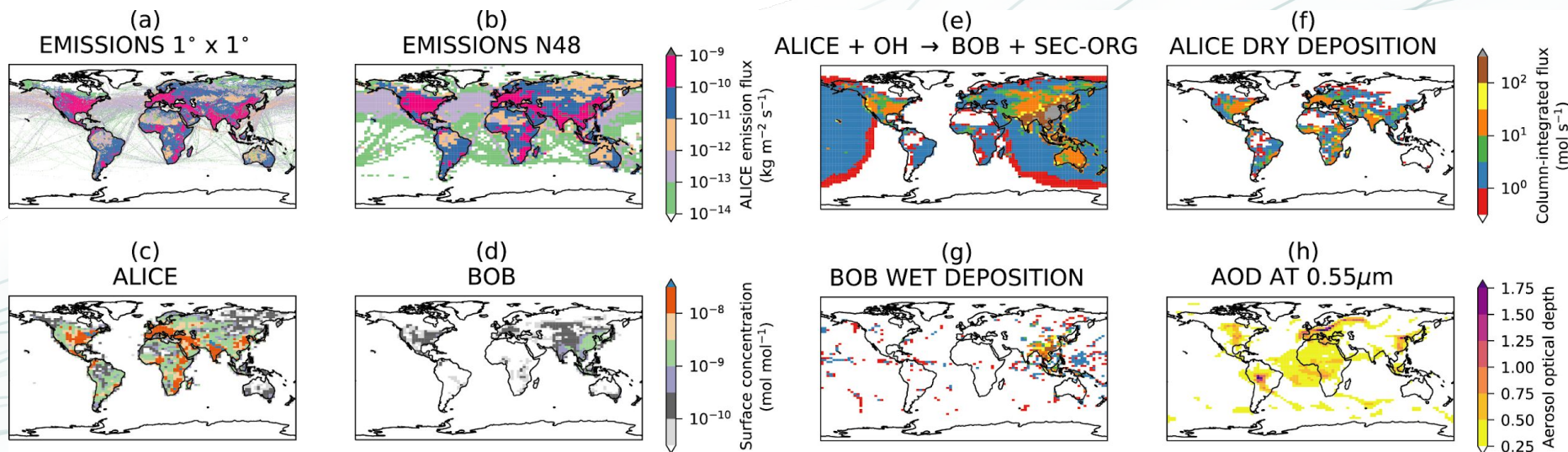
# Starting to use UKCA

- Often you will want to use UKCA to answer questions like these:
  - *What happens when I add in reaction A to form new species B?*
  - *What is the effect of changing the emissions of C?*
  - *How does the deposition of D affect process E?*
  - *How do my changes affect the aerosol properties?*
  - *What is the budget of F?*
    - *Output the fluxes of reactions G, H, and I to diagnose it.*
- When you have completed the UKCA Tutorials you should have a basic understanding how to make the required changes needed to answer these questions





## ALICE + OH $\rightarrow$ BOB + Secondary Organic Compound



# Tutorial Tasks

Despite seeming to be straight-forward, this is actually quite a big job as it involves

- UKCA code changes
  - New species
  - New emissions
  - New reactions/depositions
- Rose changes
  - Running the UKCA Box Model and the UM
  - Editing of diagnostic definition files & associated metadata changes
  - Changes to STASH (diagnostic) output
- Working with various UM files
  - Regridding input data
  - Creating NetCDF files
  - Viewing and processing UM output in Python



# Tutorial Tasks

When working with UKCA it is important to

1. Break the tasks down into manageable chunks.

This is why the task is split across multiple tutorials

2. Remember that UKCA is both a standalone model and sits within the UM framework



# Tutorial Tasks

1. The UKCA Box Model and Rose (1-2)
  - Including plotting output and adding new species and chemical reactions
2. UKCA Box Model chemistry (3-4)
  - Adding new species and reactions
3. General use of UM-UKCA and Rose (5-6)
  - These cover the basics of the copying and running a UM-UKCA suite, before outputting a field through STASH
4. Implementing your new chemistry within UM-UKCA (7-11)
  - These break down the chemistry task into smaller chunks: adding UM tracers, emissions, dry and wet deposition, and chemical diagnostics
5. UKCA Aerosols (12)
  - This covers looking at the aerosol optical depth and other quantities in more detail.
6. Plotting and processing UM-UKCA output using Python (13)
  - This tutorial makes use of both Iris and cf-python



# Tutorial Tasks

- **Things to know before you start**
- **Background and Motivation**
- **Configuring X2Go client & other connection methods**
- **Additional Resources**
- **January/February 2024 Schedule**
- **Accessing the Python notebooks**

Useful information on accounts, fcm, and suites

Framing the problem

How to connect to your computer

Recordings and handouts

What we're doing this week

How to connect to use python

#	Difficulty	Time to Complete	Topic	Video
1	EASY	Under 1 hour	Running an existing UKCA Box Model Suite	Walkthrough (YouTube)
2	MEDIUM	1-2 hours	Changing UKCA Box Model Options	Walkthrough (YouTube)
3	MEDIUM	1-2 hours	Add new UKCA chemical tracers	Walkthrough (YouTube)
4	MEDIUM	1-2 hours	Adding new chemical reactions	Walkthrough (YouTube)
5	EASY	Under 1 hour	Running an existing UM-UKCA suite	Walkthrough (YouTube)
6	MEDIUM	1-2 hours	What is STASH?	Walkthrough (YouTube)
7	HARD	2 or more hours	Adding new UKCA tracers to the UM	Walkthrough (YouTube)
8	HARD	2 or more hours	Adding emissions	Walkthrough (YouTube)
9	MEDIUM	1-2 hours	Adding dry deposition of chemical species	Walkthrough (YouTube)
10	EASY	Under 1 hour	Adding wet deposition of chemical species	Walkthrough (YouTube)
11	HARD	2 or more hours	Adding new UKCA chemical diagnostics	Walkthrough (YouTube)
12	HARD	2 or more hours	Examining Aerosol Impacts	Walkthrough (YouTube)
13	HARD	2 or more hours	Viewing and processing UKCA data with python	Walkthrough (YouTube)

The Tutorials themselves, including detailed instructions, worked solutions, and a video walkthrough.

These need to be done in sequence as each tutorial builds on the previous one.



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# Course Context

After doing these Tutorials you should

- Be more confident using Rose
- Be able to copy an existing UKCA suite, run it, and be able to understand the output
- Be familiar with STASH and working with UM output
- Be able to add new UKCA tracers
- Be able to create and add emissions into UKCA
- Be able to define new and edit existing chemical reactions
- Be able to define new dry and wet deposition of chemical species
- Be able to output new chemical diagnostics
- Be able to plot and process UKCA data





# Training VMs on AWS

You have been given your own computer to run the UKCA tutorials on.

You will need to connect to it in some way, e.g. X2Go, Terminal, or MobaXTerm.

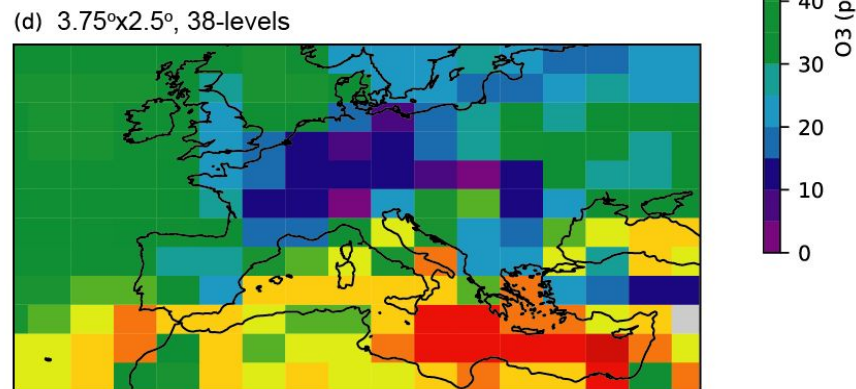
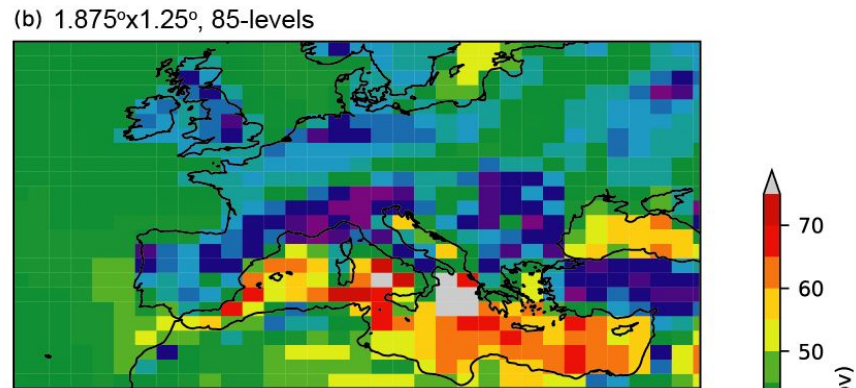
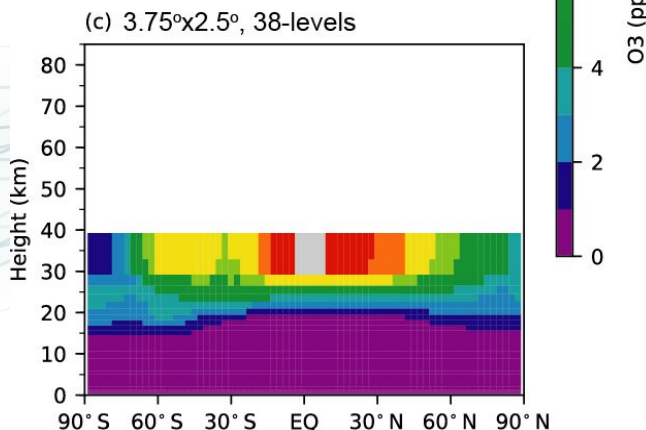
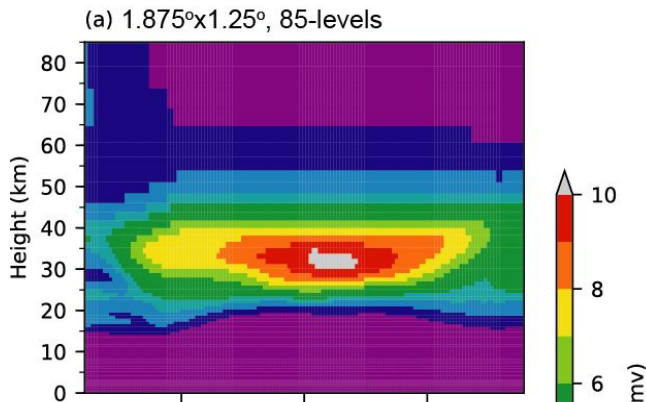
The screenshot displays a desktop environment with two main windows. The top window, titled 'X2GO-ukcatr01-50-1611739014\_stdLXDE\_dp32', shows a task manager interface with a table of tasks. The bottom window, titled 'ukcatr01@ukca-vm01: ~/cylc-run/u-cb681/work/1/atmos/pe\_output', shows a terminal window with a command prompt and output.

task	state	host	job system	job ID	T-submit	T-start	T-finish	dT-mean	latest message
1	running								
VM	running								
fcm_make	succeeded	localhost	at	1	09:20:22Z	09:20:23Z	09:21:52Z	PT1M29S	job(01) succeeded
recon	succeeded	localhost	at	2	09:21:55Z	09:21:55Z	09:22:07Z	PT12S	job(01) succeeded
atmos	running	localhost	at	3	09:22:09Z	09:22:10Z	*	*	job(01) started

```
ukcatr01@ukca-vm01: ~/cylc-run/u-cb681/work/1/atmos/pe_output
File Edit Tabs Help
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work$ ls
1
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work$ cd 1/
atmos/ fcm_make/ recon/
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work$ cd 1/
atmos/ fcm_make/ recon/
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work$ cd 1/atmos/pe_output/
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work/1/atmos/pe_output$ ls
atmos.fort6.pe0  atmos.fort6.pe1  atmos.fort6.pe.stdout
ukcatr01@ukca-vm01:~/cylc-run/u-cb681/work/1/atmos/pe_output$ tail -f atmos.fort
6.pe0
0.0000E+00
0.0000E+00
update pattern: updating coeffc and coeffs
*****
* Linear solve for Helmholtz problem
* Outer Inner Iterations InitialError FinalError
* 1 1 17 0.100000E+01 0.461313E-04
* 1 2 7 0.142479E-01 0.635002E-04
*****
Qcf < 0 fixed by PC2, ( 7 occurrences)
Qcl < 0 fixed by PC2, ( 4 occurrences)
```



**Climate  
resolution  
192x144x85  
grid points**

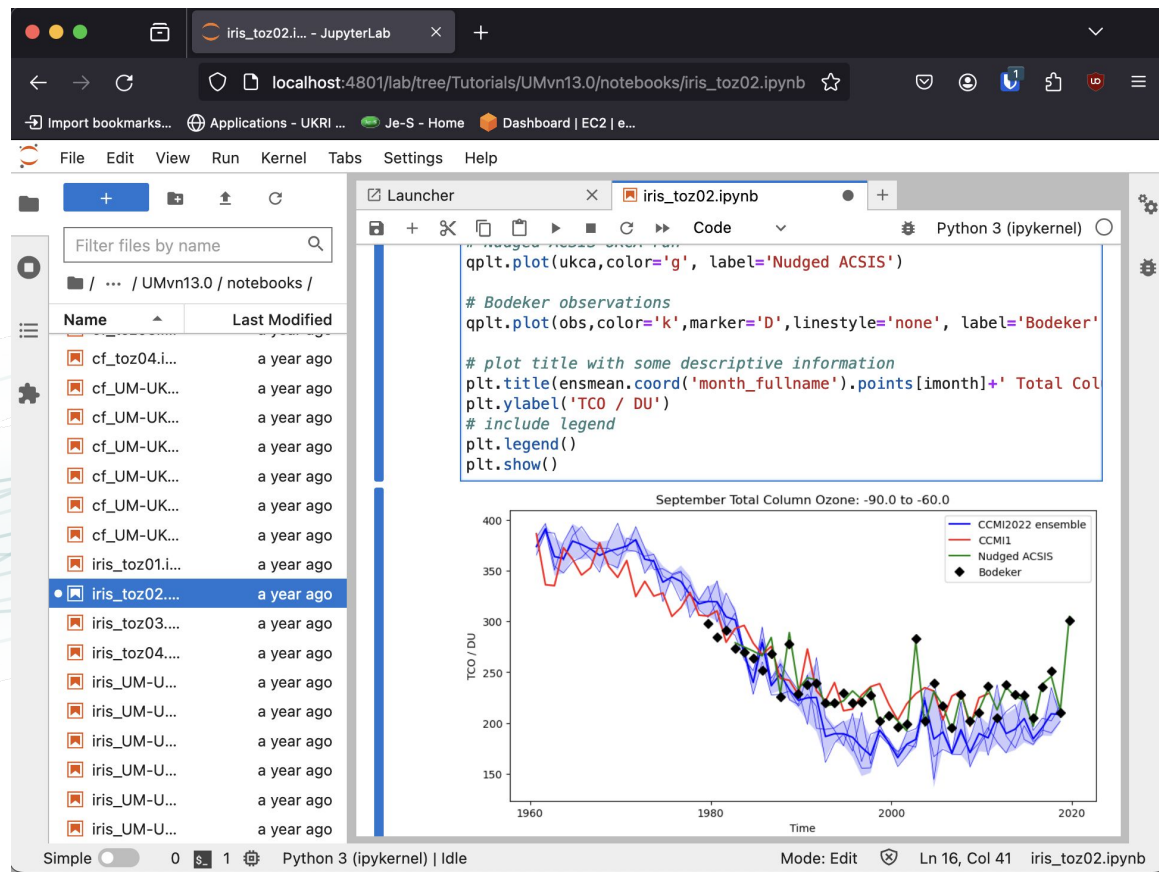


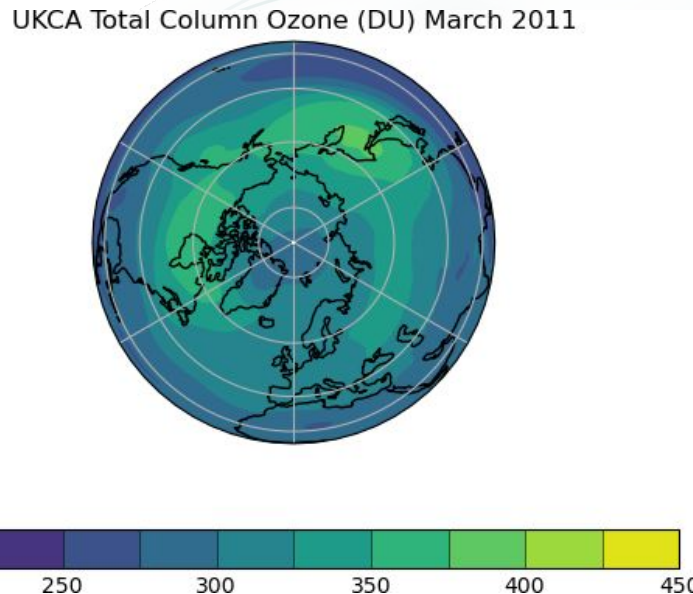
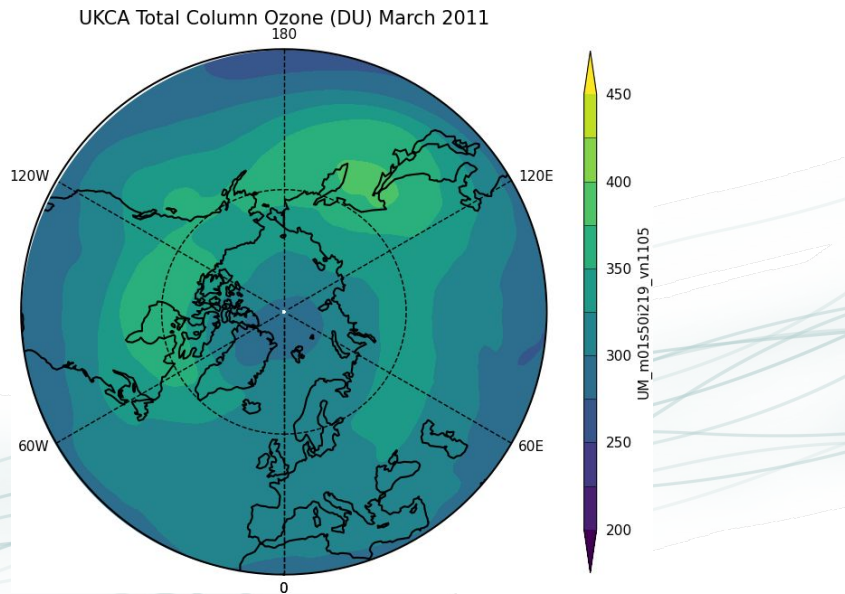
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# Python

A range of Jupyter notebooks have been prepared to aid you during the tutorials. These include plotting output from the box model, regridding and generating emissions files, and processing aerosol diagnostics, as well as working with observational and model data.

You will need to be able to set up your personal computer so that you can load the notebooks in your own web browser.





Equivalent notebooks making use of both the **cf-python** and **Iris** libraries are provided. Both basically provide the same functionality, but do things slightly differently.





# Code Management Tips and Tricks

The UKCA and UM codes as well as the Rose suites that define job configurations are all held under **version control** and are managed by a tool called **fcmm**.

Useful **fcmm** commands are given on the “Things to know before you start” page.

During these tutorials you will have several code branches and Rose suites. As all of these are under version control, so frequent use of **fcmm commit** is encouraged.

While it is probably best to use a **working copy** of a branch or suite while you are developing a change, it is best practice to commit your changes prior to doing any production runs, and move to pointing to the *repository code* within the suite, with a fixed revision number.

If you've not used version control, Rose, or the UM before - don't worry, we can discuss this further throughout the week.



# Next Steps

Now that you're all experts in UKCA, how can you get started using it?

- For PhD students and NERC-funded PDRAs at UK Universities, you should be able to get access to the PUMA service and ARCHER2 to be able to run UM-UKCA.
- If you are doing work to develop and improve UKCA, then you may be able to get access to the Monsoon2 system, provided by the Met Office.
- You will also need a JASMIN Group Workspace where you can archive and process model data.
- For developing new code, you may find the Met Office virtual machine is a good system to use.

<https://github.com/metomi/metomi-vms>



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# Next Steps

In terms of configurations to use, we recommend:

- UKESM1.0/1.1 is very well tested and documented, with a large number of existing simulations that can be analysed and used as baselines for other experiments - see the NCAS CMS website <http://cms.ncas.ac.uk/>
  - This model can also be configured so that it is “nudged” to reanalysis data, e.g. ERA-5, to give a better representation of past conditions.
- We also provide the UKCA AMIP Development Suite - this is a year-2000 timeslice (free-running or nudged) that can be used when developing new code for inclusion in the UKCA trunk.
- A 2-day Short Testing suite is also provided so that you can quickly test new code changes. This runs your code through 3 different chemistry schemes, performs robustness checks, and with different compiler options.
- For running the UKCA Box Model, you will need to use the virtual machine.
- See the **Support** section of the UKCA website



# Study with the National Centre for Atmospheric Science



## Fundamentals

- Get started with atmospheric science
- Put Linux shell and Python into practice
- Use the JASMIN supercomputer



## Making Measurements

- Plan and design experiments
- Link measurements to models
- Work with radar data
- Explore practical aerosol science



## Modelling

- Become a proficient user of climate models
- Operate the UK Chemistry Aerosol (UKCA) Model
- Make the most of the Unified Model
- Apply the Model for Prediction Across Scales – Atmosphere (MPAS-A)

# Your future development

**Keep up to date with NCAS' upcoming training courses:**

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Subscribe to the monthly NCAS newsletter / training course mailer

Follow NCAS on social media

Email [training@ncas.ac.uk](mailto:training@ncas.ac.uk)



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# Acknowledgments

Many thanks to the demonstrators who are helping out during this course:

Many thanks to the Software Sustainability Institute for supporting this training.

Many thanks to those at AWS for their help and support in setting up the infrastructure.



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# Any Questions?



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