



Natural  
Environment  
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Software  
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Institute



UNIVERSITY OF  
CAMBRIDGE

# Introduction to UKCA

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## Practicals

- The Practical make use of both the UKCA box model and the Unified Model using the Rose & Cylc interface at UM vn13.0
- There are a number of differences between these and some previous versions of the practicals that you may have seen
- The Tutorial jobs are a cut-down configuration designed for training and testing, so may be different to suites you run as part of your research

## Using UKCA

- What resources are available?
  - UKCA Evaluation Suite
  - NCAS Computational Modelling Services
  - Met Office Science Repository Service
    - Provide access to the UM source code and suites used to run the UM
    - UM & UKCA wiki pages give lots of information regarding the development process
    - A full set of UM Documentation Papers are available
    - <https://code.metoffice.gov.uk/trac/um>
    - <https://code.metoffice.gov.uk/trac/ukca>

## What Resources are Available?

You've decided 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 over-come and solve model problems.

## What Resources are Available?

- The UKCA Tutorials have been developed to address this first problem
  - A UKCA Evaluation Suite is available on the Met Office desktops, Monsoon2, & JASMIN

[http://www.ukca.ac.uk/wiki/index.php/Evaluation\\_suite2](http://www.ukca.ac.uk/wiki/index.php/Evaluation_suite2)

- The second issue is addressed by the NCAS Computational Modelling Services (CMS) team based in Reading

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

# UKCA Evaluation Suite

- A UKCA Evaluation suite has been developed by Mohit Dalvi at the Met Office
- Takes existing scripts developed by the different groups developing UKCA and combines them in a single package
- UM-UKCA climate jobs output a set of standard diagnostics which are then read by the suite to produce a series of plots to aid model evaluation
- In the Met Office additional tools such as AutoAssess and ValNote are available, but the UKCA Evaluation Suite is also available on JASMIN





# UKCA Evaluation Suite

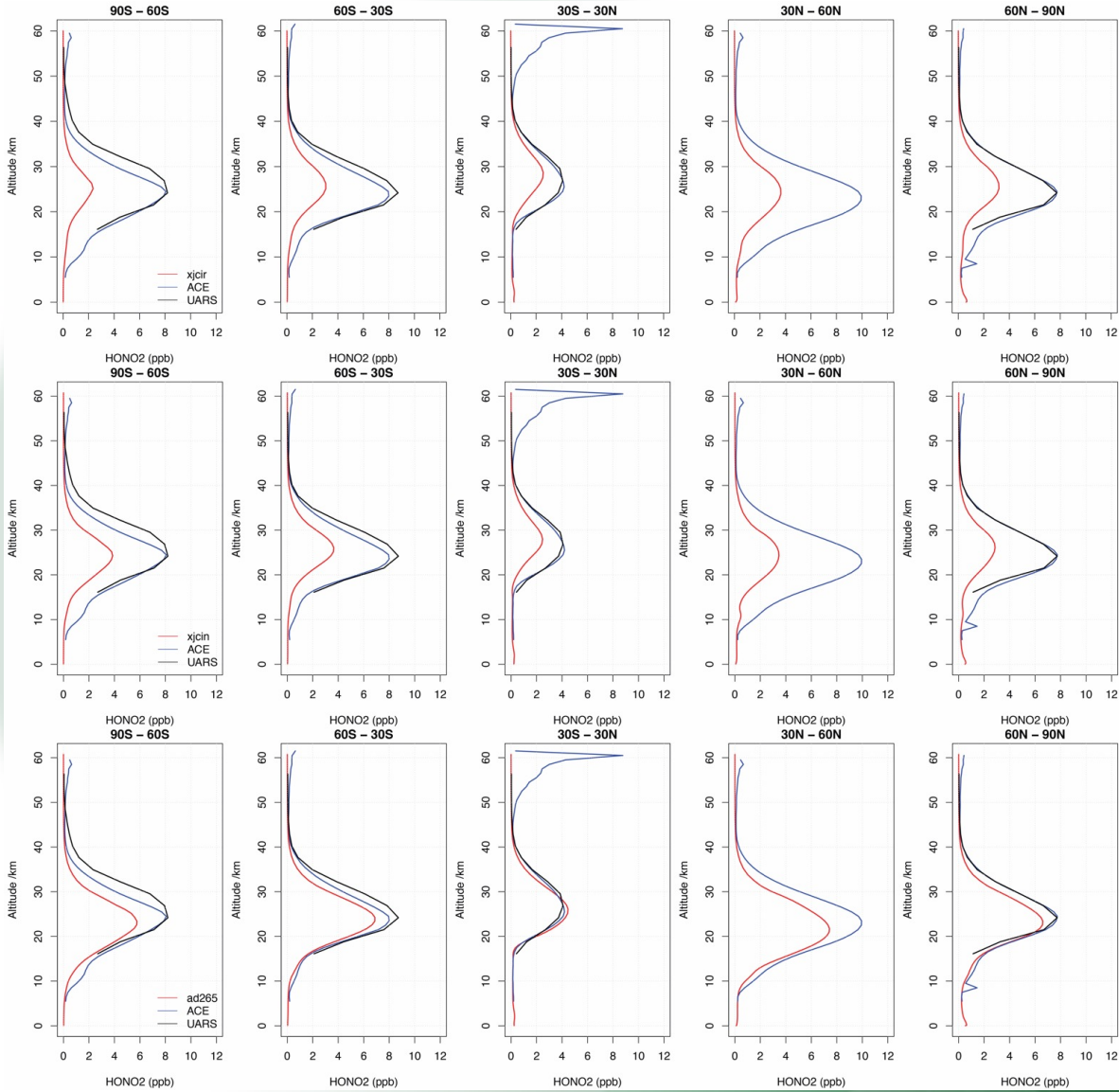
NO<sub>y</sub>

Age  
of Air

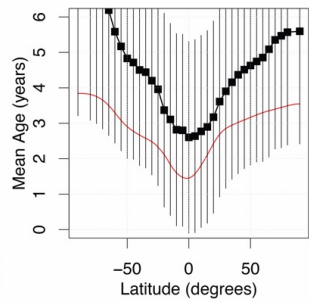
vn7.3  
HadGEM3-A  
r2.0 N48L60

vn8.4  
GA4.0

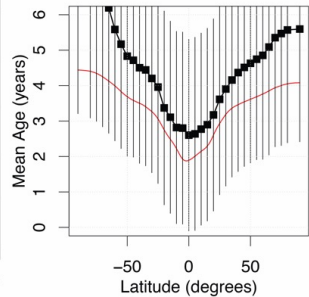
vn10.3  
GA7.0



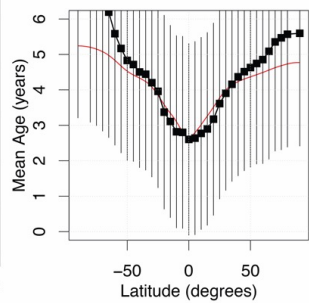
Mean Age, 23km (~50hPa)



Mean Age, 23km (~50hPa)



Mean Age, 23km (~50hPa)



## What do CMS do?

- CMS provide the PUMA service. This runs the UMUI & Rose/Cylc servers which are used to submit UM jobs to ARCHER2
- They provide UM training, both as an on-line FCM tutorial and as a 2-day workshop
- They provide tools, such as Xconv and Xancil, the cf-python and cf-plot python libraries, and cf-view
- They manage the NERC atmospheric group on ARCHER2 (n02)
- They provide the **CMS Helpdesk**





# CMS Modelling Helpdesk



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[all tags ▸](#)

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Topic

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Activity

## 🚩 Welcome to the NCAS-CMS Modelling Support Forum

Welcome to the CMS Modelling Support Forum. Here you can raise all your modelling support queries (topics) covering Unified Model, NEMO, problems logging into supported platforms like ARCHER2, etc. Before raising a que... [read more](#)



0

422

Jun '21

## Unable run rose suite

[ARCHER2](#)



8

27

2h

## Support for MONC?



12

33

3h

## Archer2 Disk Quota Exceeded

[Unified Model](#)

[ARCHER2](#)



0

6

17h

## Reconfiguration fails with 2022 analysis files (UM vn12.0 nested suite)

[Unified Model](#)

[Monsoon2](#)



10

75

1d

## Configuring PPTransfer with GridFTP

[Unified Model](#)

[ARCHER2](#)



6

15

1d

## Perl script not running on pumanew



1

7

1d



Premise:

**What are the most common things that a PhD student or Researcher 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



## Tutorial Tasks

Through-out the tutorial you are asked to perform a series of tasks. In fact, these are mostly part of one big task which is:

**Create two new species, ALICE and BOB, then add in emissions of ALICE and the reaction**



**(with Sec\_Org included if you are using GLOMAP-mode aerosols) before adding in the dry deposition of ALICE and the wet deposition of BOB. You should also output the fluxes through the reaction and deposition processes.**

**Later you will look at several aerosol diagnostics.**

## Tutorial Tasks

- Despite seeming to be straight-forward, this is actually quite a big task as it involves
- UKCA code changes
  - New species
  - New/editing reactions & deposition
- UM-UKCA code changes
  - New emissions
- Working with various UM files
  - Regridding input data
  - Creating NetCDF files
  - Processing UM output



## Tutorial Tasks

- Despite seeming to be straight-forward, this is actually quite a big task as it involves
- Rose changes
  - Changing configuration settings
  - Editing of STASHmaster\_A (UM diagnostic definition) file & associated metadata changes
  - Changes to STASH (diagnostic) output

When working with UKCA it is important to  
Break the tasks down into manageable  
chunks



## Tutorial Tasks

The Tutorials are broken down into five sections

### 1. General use of the UKCA Box Model and Rose (Tutorials 1-2)

- These tutorials cover the basics of the copying and running a UKCA Box Model suite, before changing various options and viewing output.

### 2. UKCA Box Model Chemistry (Tutorials 3-4)

- Here we add new species and reactions in the UKCA Box Model and test with different configurations.



## Tutorial Tasks

The Tutorials are broken down into five sections

### 3. UM-UKCA Chemistry (Tutorials 5-11)

- Here we also cover the basics of the copying and running a UM-UKCA suite, before outputting a field through STASH
- Adding tracers
- Adding emissions
- Adding dry and wet deposition
- Adding chemical diagnostics

## Tutorial Tasks

The Tutorials are broken down into five sections

### 4. UM-UKCA Aerosols (Tutorial 12)

- The aerosol tutorial covers looking at the aerosol optical depth and other quantities in more detail, as well as performing sensitivity experiments

### 5. Working with UKCA data (Tutorial 13)

1. Here we use the Iris and cf python libraries to look at UKCA and observational data


## Tutorial Tasks

These tutorials have been designed so that you can go through them in your own pace and in your own time

This is partly because some people will work at different rates.

# The Tutorials

## Connecting

1. Turn on your desktop and select **MCS Linux**
2. Login using your provided username and password, e.g. **v2340**
3. Open a terminal, e.g. by pressing the Windows key and clicking the icon 
4. Type **ssh -X ukca** and press return

This will log you in to the computer that you will use for the Tutorials.



You are now connected to a virtual machine on the AWS cloud that has all the necessary software installed for the course

1. To start Jupyter on the UKCA instance, enter either `"jlab &"` or `"jnotebook &"`
2. On the desktop, open a new terminal and enter `jopen`
3. Open **Firefox** and go to `http://localhost:4801/?token=UKCATraining`

# **Tutorial 1:**

## **Running an existing UKCA Box Model suite**



## Tutorial I

This tutorial is designed to make you more familiar with Rose and the directory structure used for UKCA and UM jobs

In this tutorial you are asked to run your copy of the Tutorial base Box Model suite, and examine the output

**rosie copy u-cq774**

Then go to your **roses/** directory to find the new suite

**You should now work through the**

**1) Running an existing UKCA Box  
Model suite**

**tutorial**

# **Tutorial 1: Running an existing UKCA Box Model suite**

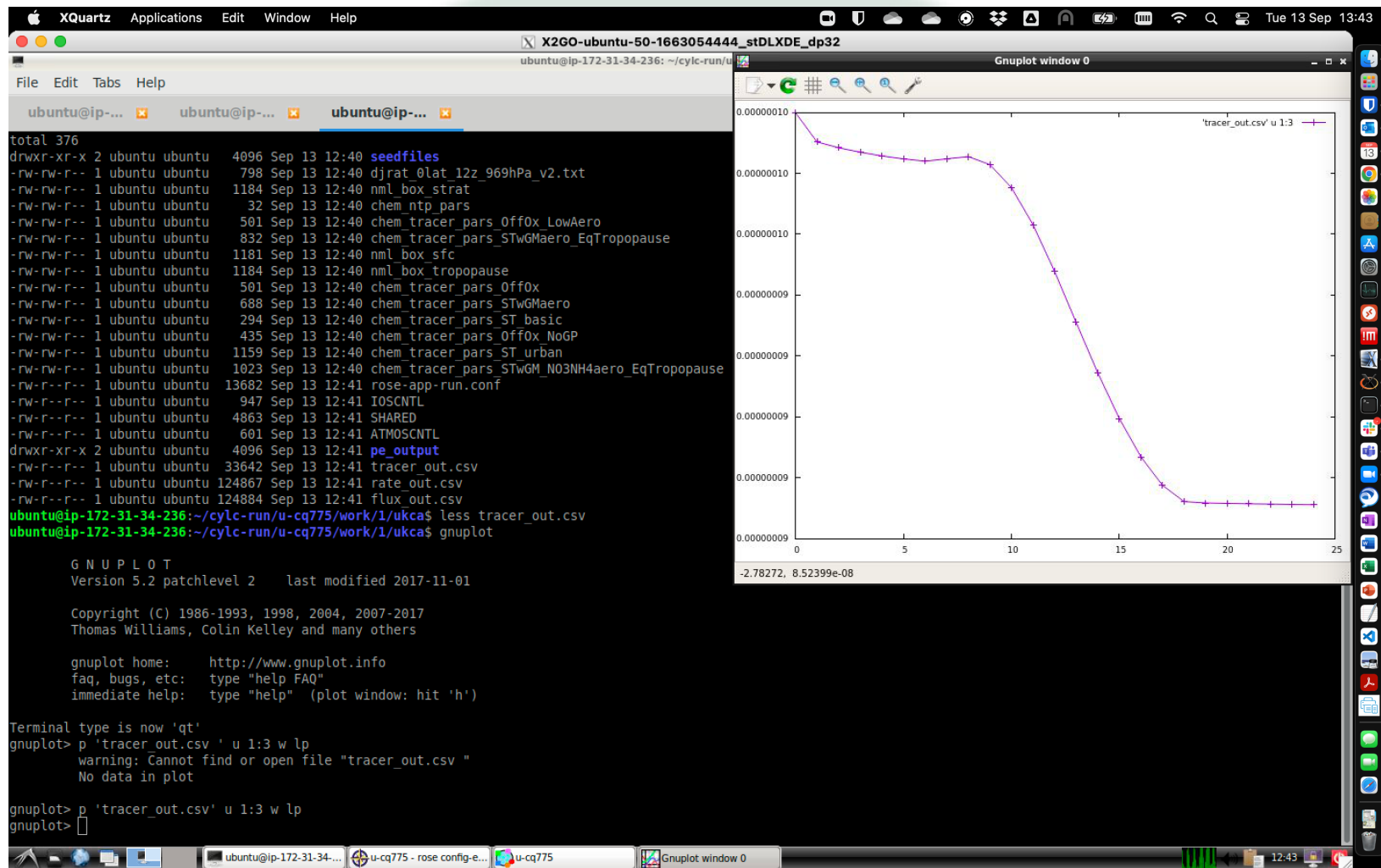
# Tutorial I

## Points to remember

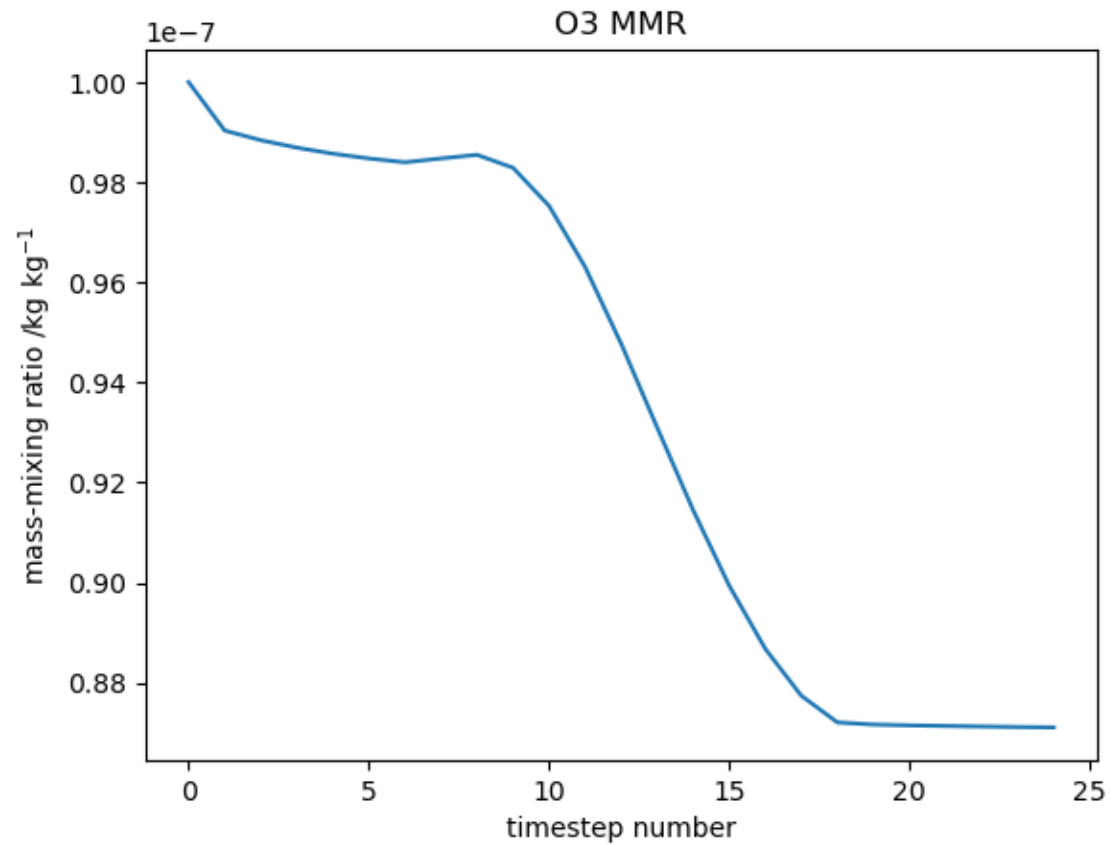
1. Messages are held in the output `job.out` and `job.err` files
2. Use the `rosie` and `rose` commands to open, edit and run jobs
3. GNUplot and/or Python can be used to look at the UKCA output



# Tutorial I



# Tutorial I



# **Tutorial 2:**

## **Changing UKCA Box Model options**

## Tutorial 2

- This tutorial is designed to make you more familiar with changing the various initial conditions for tracers and environmental conditions within Rose
- You will also change the run length and chemical scheme used, as well as turning on and off the GLOMAP-mode aerosol scheme



**You should now work through the**

**2) Changing UKCA Box Model options**

**tutorial**

# **Tutorial 2: Changing UKCA Box Model options**



## Tutorial 2

### Points to remember

1. Changing the time settings of the box model requires changing `model_basis_time`, `run_target_end`, `steps_per_periodim` and `chem_timestep`
2. Environmental and tracer conditions are set using `ukca_box_nml` and `tracer_in_filename`
3. The chemistry and aerosol schemes are controlled using `i_ukca_chem` and `l_ukca_mode`, remembering to turn off aerosol and stratospheric heterogeneous chemistry with `l_ukca_chem_aero` and `l_ukca_het_psc`.



# **Tutorial 3:**

## **Adding new chemical tracers**



## Tutorial 3

- Here you will start to learn about making new code branches on MOSRS
- Once you have your branch, you can then make the required code changes and include this branch in your Rose suite so that these changes are then picked-up and included in your box model runs.

**You should now work through the**

**3) Adding new chemical tracers**

**tutorial**

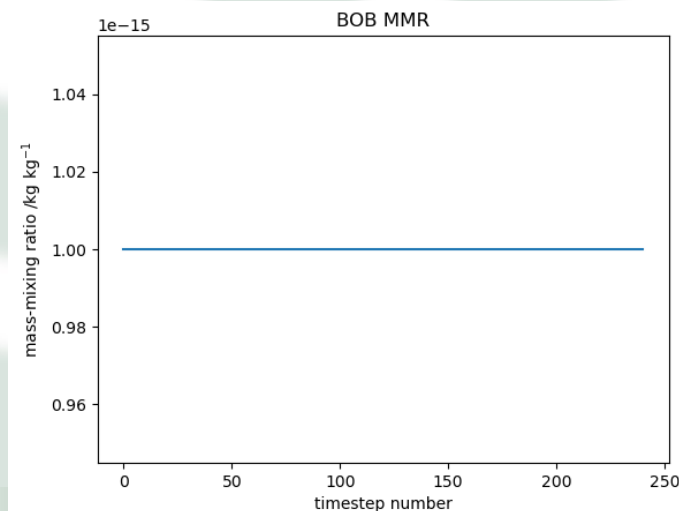
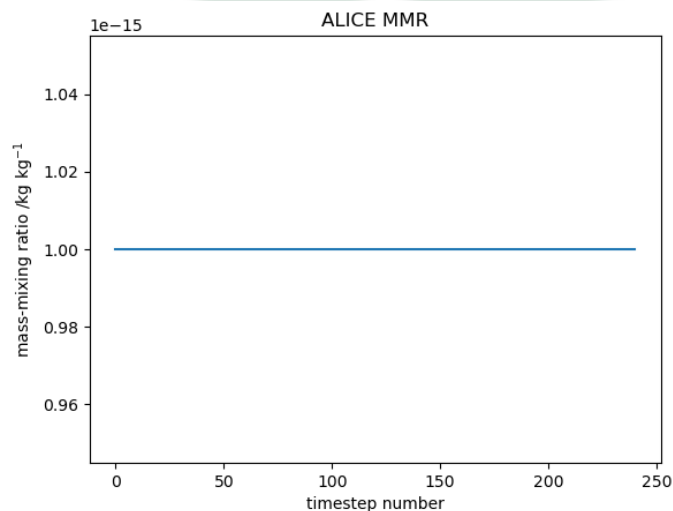


# **Tutorial 3: Adding new chemical tracers**

# Tutorial 3

## Points to remember

1. As well as defining your new chemical tracers within `ukca_chem_master.F90`, you will also need to define the conversion factors from VMR to MMR with `ukca_constants.F90` and `ukca_cspecies.F90`.
2. If there are no reactions associated with these species, their concentrations will not change



# **Tutorial 4:**

## **Adding new chemical reactions**



## Tutorial 4

In this tutorial you are taught about the different types of reactions UKCA considers

- a) Bimolecular reactions
- b) Termolecular reactions
- c) Heterogeneous reactions
- d) Photolysis reactions

The format of how these reactions are defined within the UKCA chemistry scheme specification module are very similar

However, special code may need to be added for some reactions





## Tutorial 4

In this tutorial you are asked to add the following bimolecular reaction



(where Sec\_Org is only included if using aerosol chemistry) using the following rate coefficients

$$k_0 = 2.70 \times 10^{-11}$$

$$\alpha = 0.00$$

$$\beta = -390.0$$

You should:

Make your changes to the UKCA chemistry specification module



**You should now work through the**

**4) Adding new chemical reactions**

**tutorial**

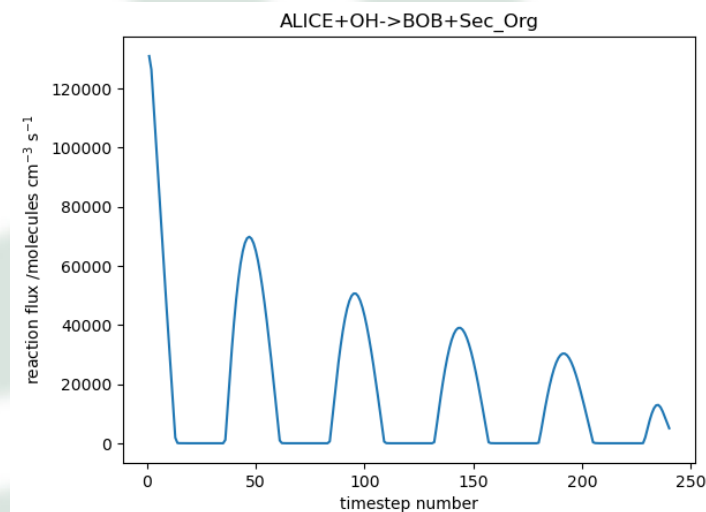
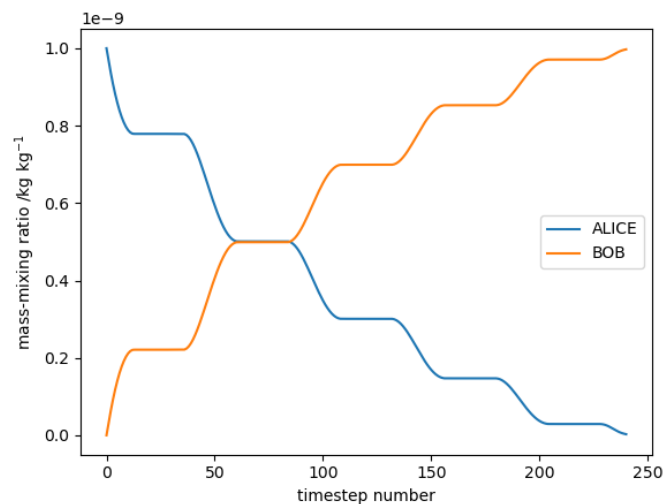


# **Tutorial 4: Adding new chemical reactions**

# Tutorial 4

## Points to remember

1. Check that you have your array sizes correct – it can be difficult to keep track
2. Once you change the initial conditions of ALICE and BOB you will be able to see the reaction progress



# **Tutorial 5:**

## **Running an existing UM-UKCA suite**

## Tutorial 5

Now that we have our new tracers and reactions within UKCA we can move to using these in a larger model, in this case the Unified Model.

Now we will take a copy of the UM-UKCA base suite, run it, and examine the output.

```
rosie copy u-cq986
```

Then go to your **roses/** directory to find the new suite

**You should now work through the**

**5) Running an existing UM-UKCA suite**

**tutorial**

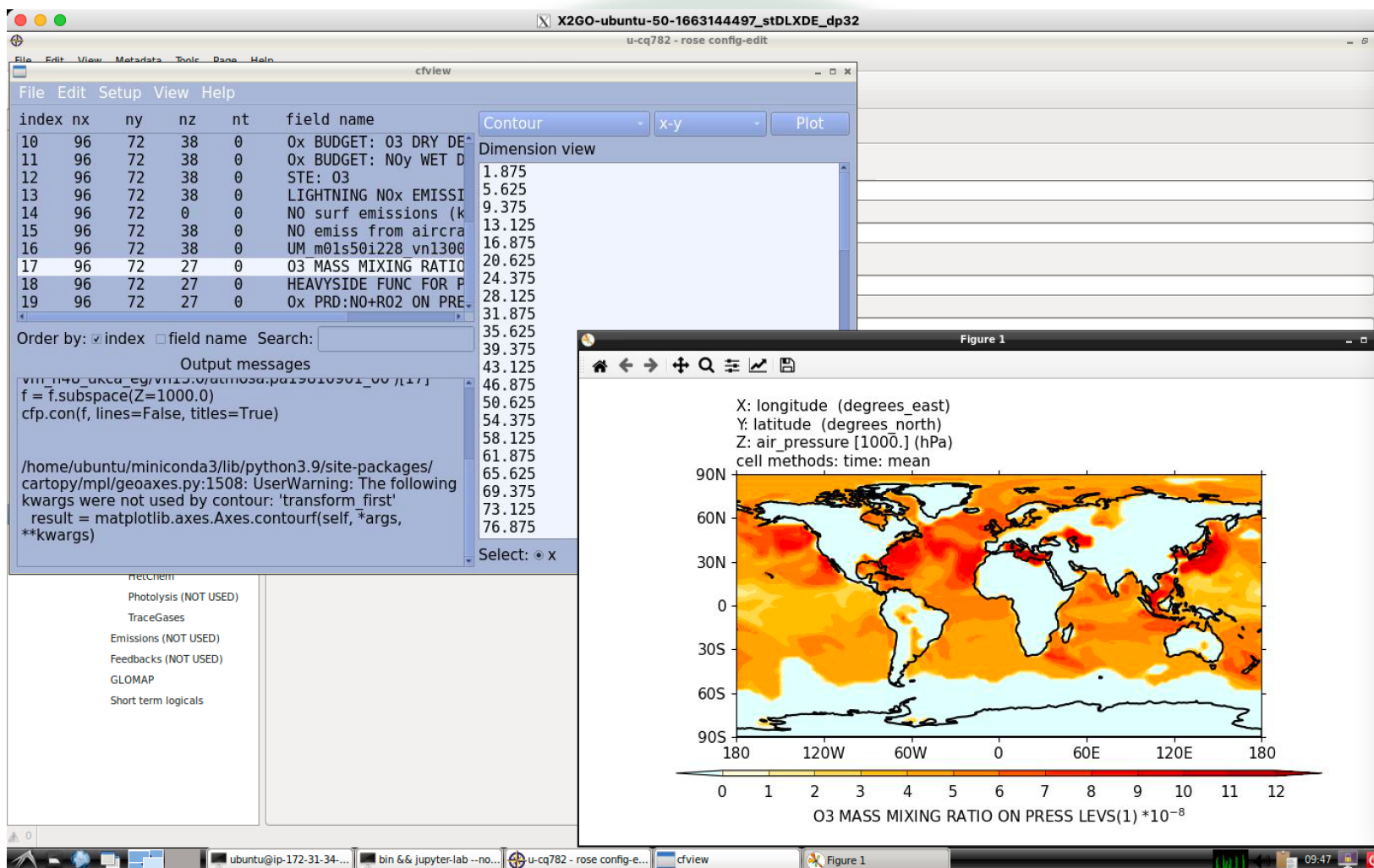
# **Tutorial 5: Running an existing UM-UKCA suite**



## Tutorial 5

- You can use the Rose search function to find things
- You can use Xconv or cf-view to view the output

# Tutorial 5



# **Tutorial 6: What is STASH?**



## Tutorial 6

- This tutorial is designed to give you an overview of the STASH panel, which is used to output diagnostics from the UM
- Some further details to do with STASH, such as making new STASH specification files, are covered in later tutorials
- You are asked to add some output and check that this is being done correctly

**You should now work through the**

**6) What is STASH?**

**tutorial**

# **Tutorial 6: What is STASH?**

## Tutorial 6

From this tutorial I hope that you have more of an understanding of what STASH can and can't do, as well as things to try if you are having problems

### Points to remember

1. Remember the undo button if you make any mistakes. Also, if you don't immediately commit changes to the repository you can easily go back to a working version
2. Remember to run the **TidyStashTransform** macro after any STASH changes
3. Xconv or cf-view can be used to take a quick look at UM/UKCA output, as well as converting this output to other formats, e.g. NetCDF



# **Tutorial 7:**

## **Adding new UKCA tracers to the UM**



## Tutorial 7

When you move to working with the UM you now need to create your tracers within the UM so that they can be transported around.

This involves code making new slots in STASH for these tracers, before adding code to tell the UM and UKCA where to find these tracer slots.

**You should now work through the**

**7) Adding new UKCA tracers to the UM**

**tutorial**



# **Tutorial 7: Adding new UKCA tracers to the UM**

## Tutorial 7

# Points to remember for the UM changes:

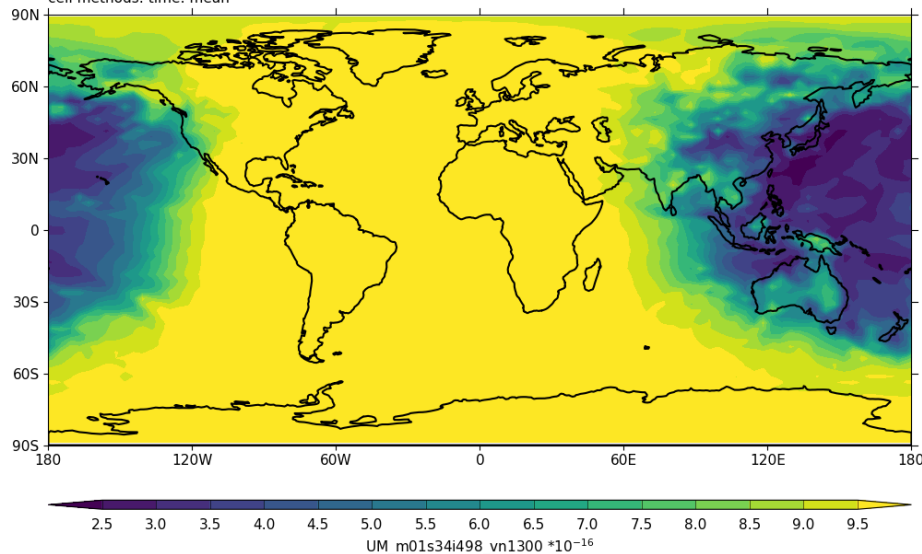
1. The total number of transported tracers is different from the number of species that UKCA considers
  - The UM is concerned with how many tracers are transported in section 34
  - UKCA is concerned with how many species, which are involved in the chemical mechanism, are transported (& how many are not)
  - This means that the UKCA diagnostic tracers, e.g. age of air appear in the STASH panel but not the UKCA species list, and H<sub>2</sub>O appears in the UKCA species list but not in STASH (as it is not transported in section 34).
2. As the UM outputs tracers in mass-mixing ratio, but UKCA performs the chemistry in volume-mixing ratio. This is why you needed to define a conversion factor for your new tracers



## Tutorial 7

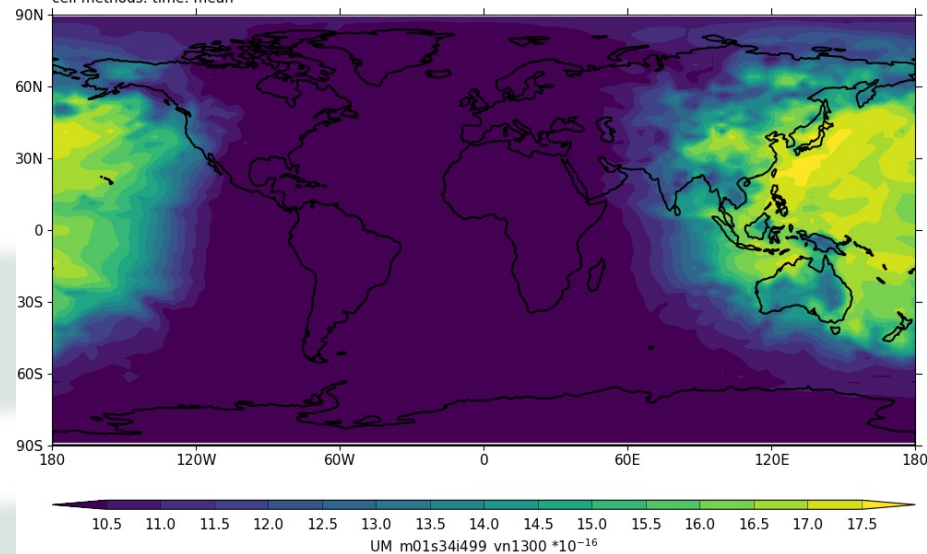
As we have already included the chemical reaction between ALICE and BOB, we can see structure in these tracers once all the linkages to UKCA are in place

X: longitude (degrees\_east)  
Y: latitude (degrees\_north)  
Z: atmosphere\_hybrid\_height\_coordinate [0.0004714]  
cell methods: time: mean



ALICE

X: longitude (degrees\_east)  
Y: latitude (degrees\_north)  
Z: atmosphere\_hybrid\_height\_coordinate [0.0004714]  
cell methods: time: mean



BOB

# **Tutorial 8: Adding emissions**



## Tutorial 8

In this tutorial you are taught about

- How to regrid emissions to the correct UM grid, include the correct metadata, and then save this as a NetCDF file with the required metadata

- How to make the necessary changes to the UKCA code

- Make changes to your suite to include this new file

You are asked to take an emissions dataset for ALICE and regrid it to N48e resolution and then use this in UKCA

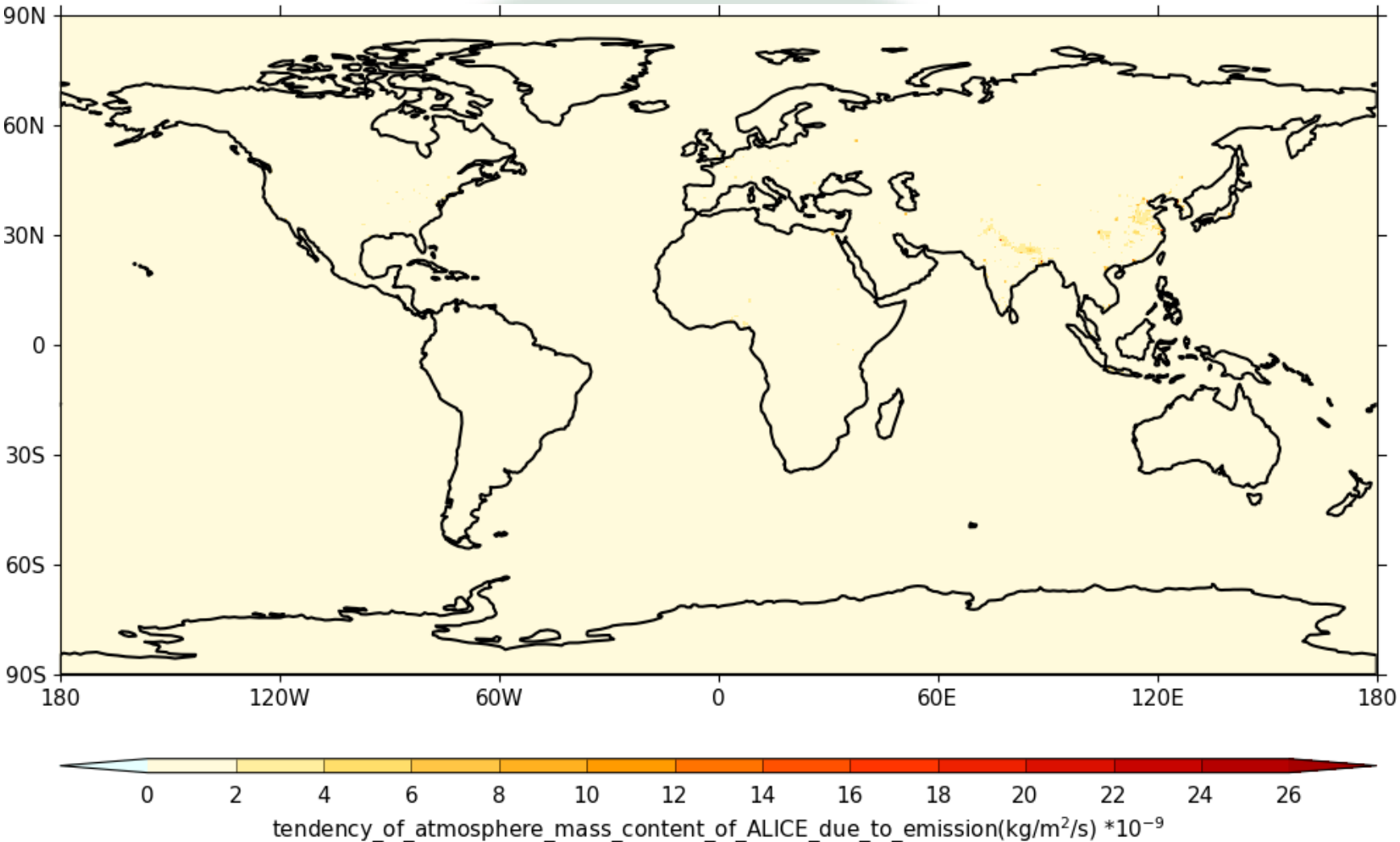
**You should now work through the**

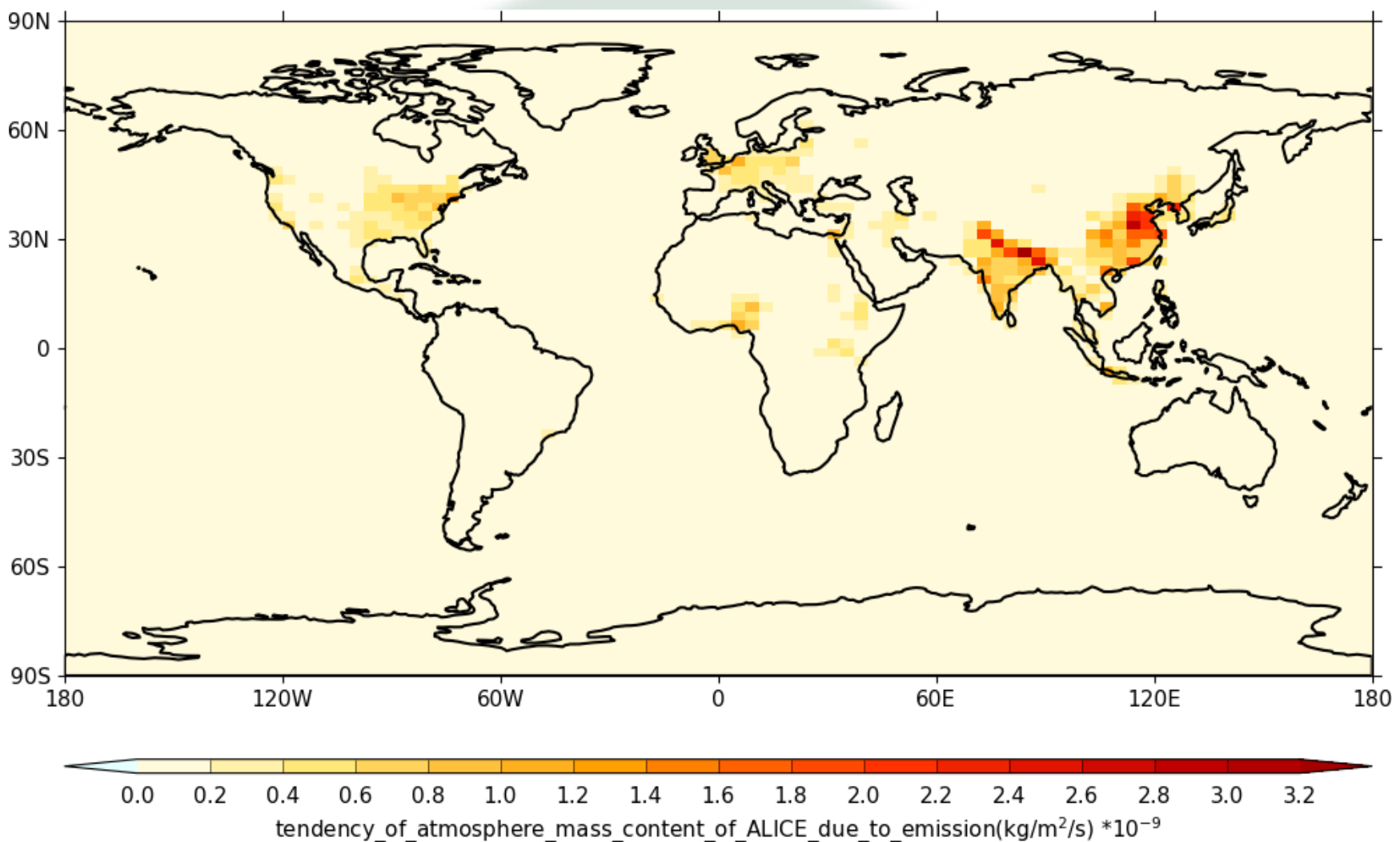
**5) Adding emissions**

**tutorial**



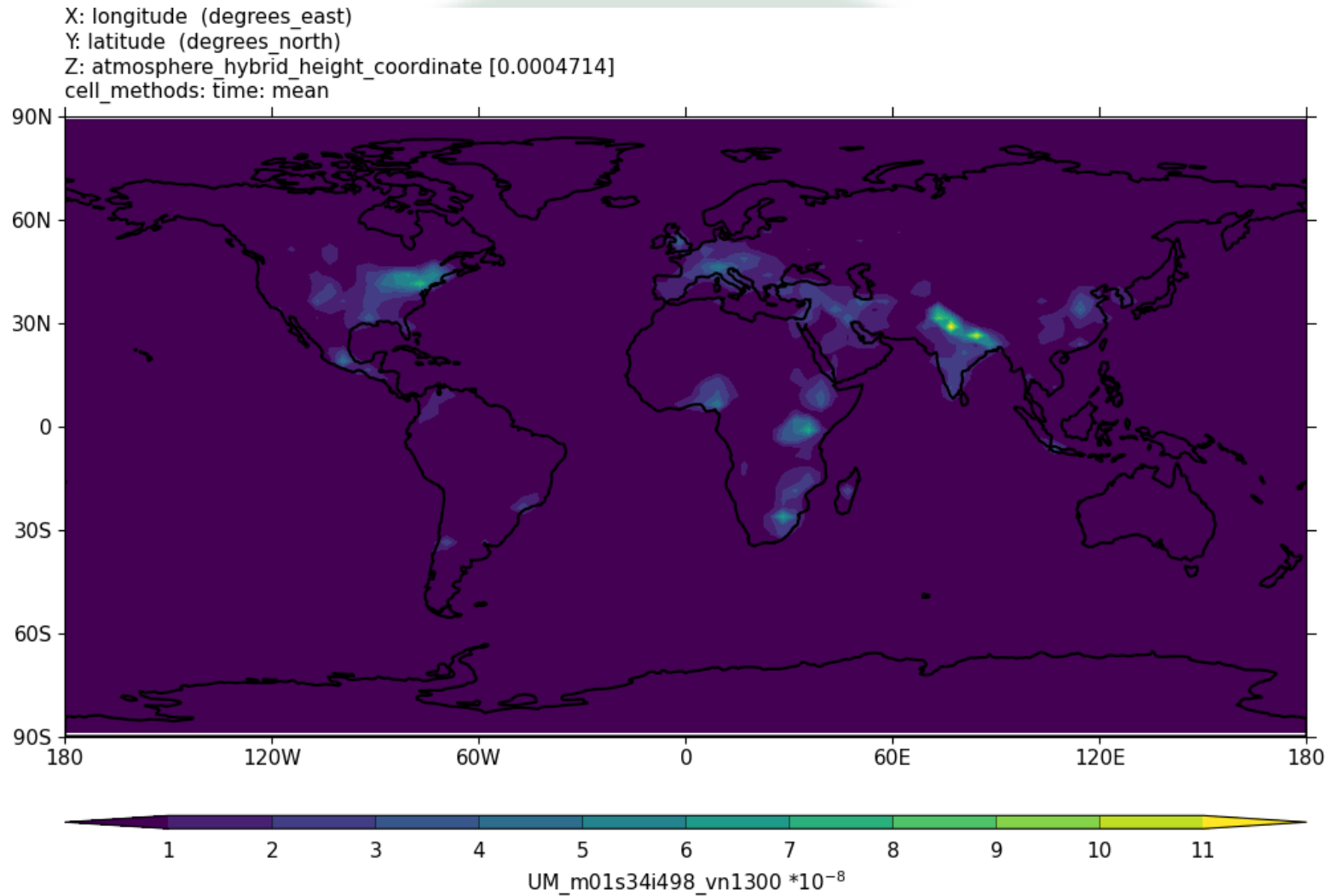
# **Tutorial 5: Adding emissions**





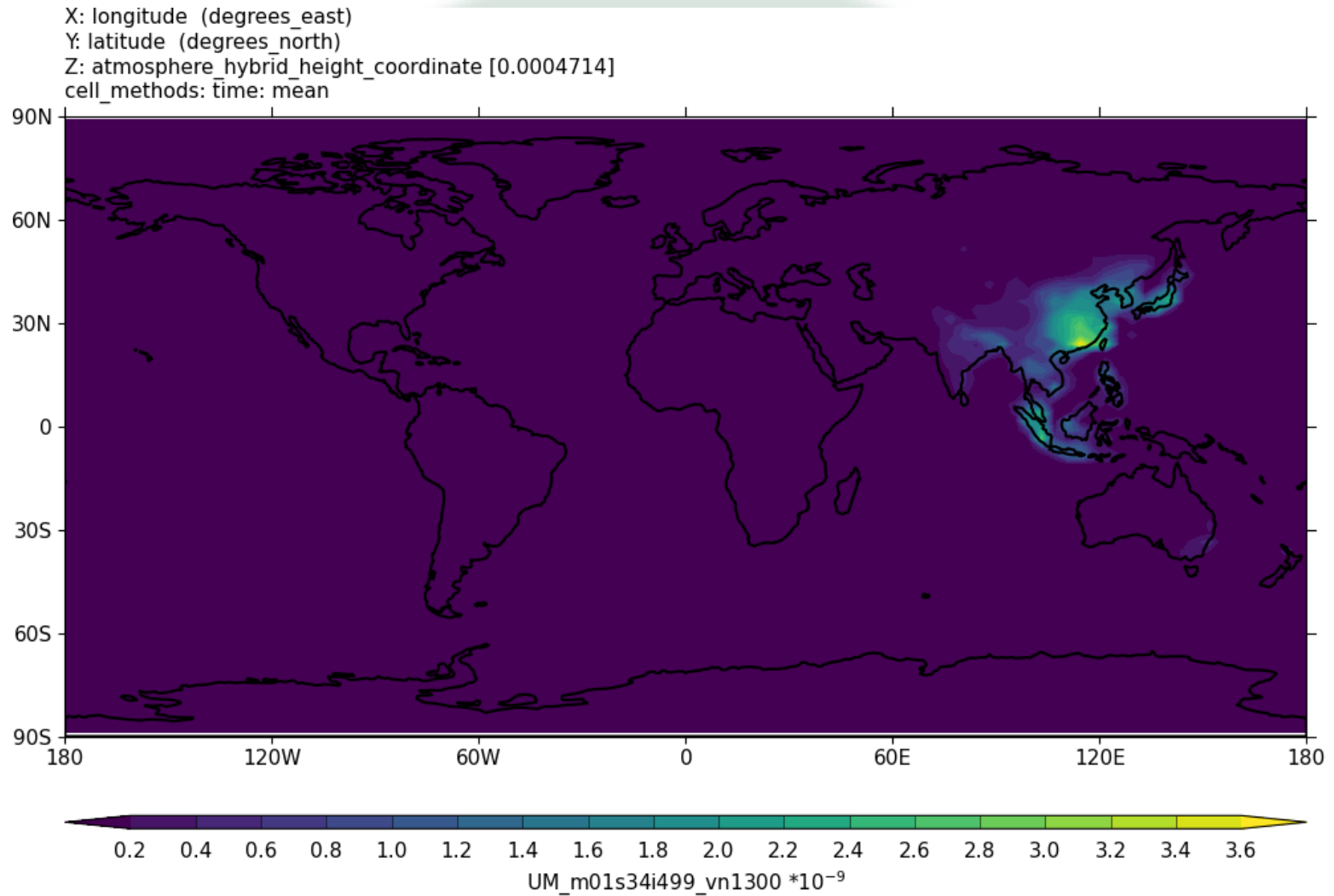
# Tutorial 8

ALICE



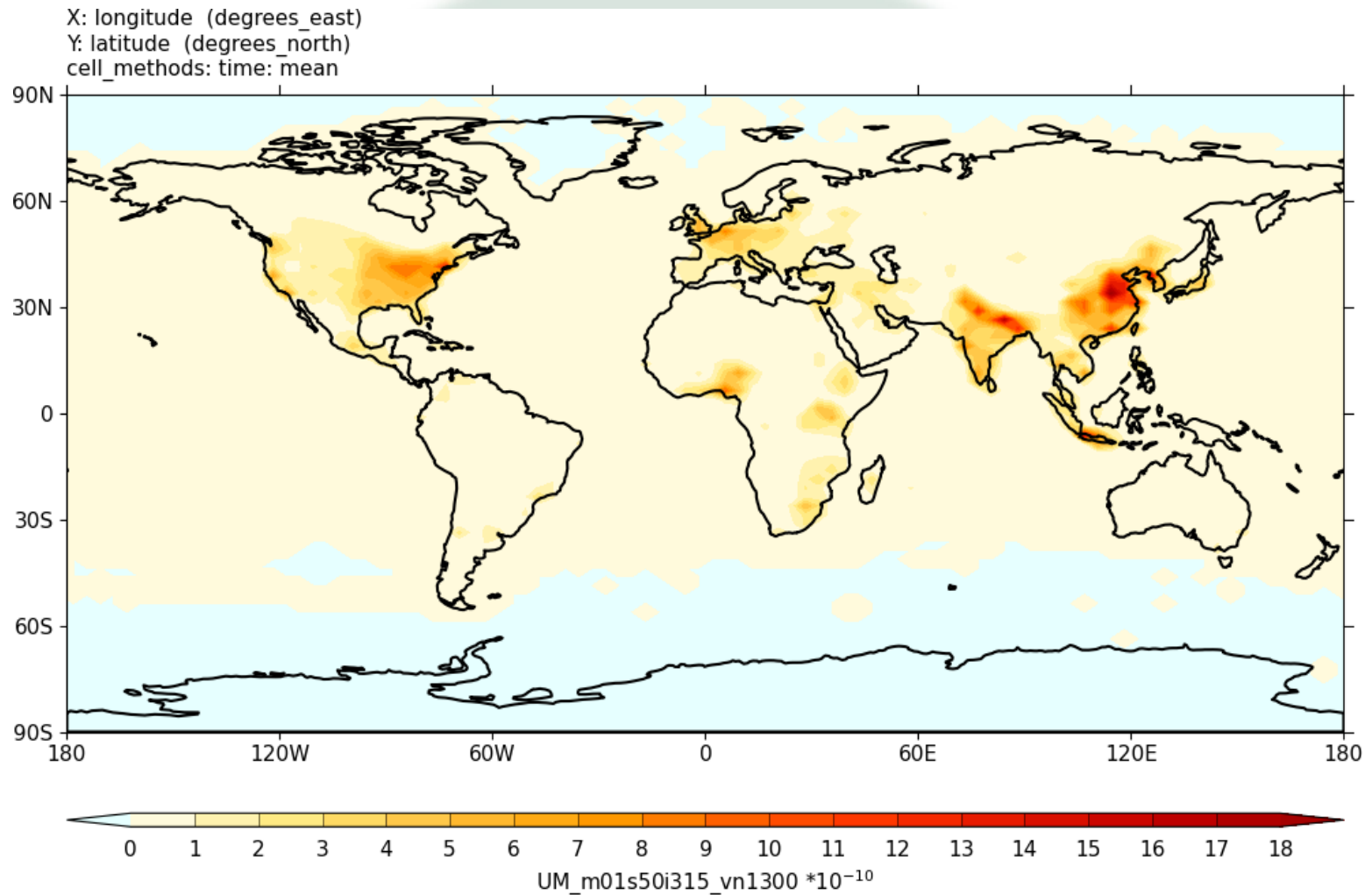
# Tutorial 8

BOB



# Tutorial 8

Reaction flux



### Points to remember:

1. You should always regrid your emissions using **area-weighted** interpolation to ensure that the same mass is emitted at the new resolution
2. You should consider the correct **metadata** settings required for your input netCDF file
3. You will also need to define the molar mass of the species being emitted into
4. You will need to make new emissions diagnostics for any new species you emit into



# **Tutorial 9: Adding dry deposition of chemical species**



## Tutorial 9

There are two dry deposition schemes that UKCA uses

1. A simple 2-dimensional scheme
2. An interactive parameterisation, based on the Wesely scheme, which deposits from throughout the boundary layer

The 2D scheme only requires changes to the UKCA chemistry scheme specification module

The Interactive scheme also requires changes to two UKCA routines

You also need to define the molar mass of the dry deposited species

## Tutorial 9

In this tutorial you are asked to add-in the dry deposition of ALICE (which deposits in the same in the same way as CO)

The values for the 2D scheme are

	<i>Summer (day)</i>	<i>Summer (night)</i>	<i>Summer (24h av)</i>	<i>Winter (day)</i>	<i>Winter (night)</i>	<i>Winter (24h av)</i>
<i>Water</i>	0.0	0.0	0.0	0.0	0.0	0.0
<i>Forest</i>	0.3	0.3	0.3	0.3	0.3	0.3
<i>Grass</i>	0.3	0.3	0.3	0.3	0.3	0.3
<i>Desert</i>	0.3	0.3	0.3	0.3	0.3	0.3
<i>Ice</i>	0.0	0.0	0.0	0.0	0.0	0.0

The values for the interactive scheme should be taken from how CO is treated in `ukca_aerod` and `ukca_surfdrr`, taking the different molecular mass of ALICE into account

**You should now work through the**

**9) Adding dry deposition of chemical species**

**tutorial**



# **Tutorial 9: Adding dry deposition of chemical species**

## Tutorial 9

### Points to remember

1. Even if you are using the Interactive scheme, you will also need to make changes to the 2D scheme
2. When adding species to the Interactive scheme you may also need to define the molar mass of the deposited species
  - Remember that there are options for 9, 13, 17, & 27 surface types

# **Tutorial 10:**

## **Adding wet deposition of chemical species**



## Tutorial 10

There is only one wet deposition scheme used in UKCA for chemical species

You will need to define the Henry's Law coefficients for each species that is wet deposited

To add in new wet deposition, you will only need to make changes to the chemistry scheme specification module

In this tutorial you are asked to add-in wet deposition of BOB using the following values

$$k(298) = 0.21 \times 10^6$$

$$-(\Delta H / R) = 0.87 \times 10^4$$

$$k(298)_{1stDissociation} = 0.2 \times 10^2$$

$$-(\Delta H / R)_{1stDissociation} = 0.0$$

$$k(298)_{2ndDissociation} = 0.0$$

$$-(\Delta H / R)_{2ndDissociation} = 0.0$$



**You should now work through the**

**10) Adding wet deposition of chemical  
species**

**tutorial**





# **Tutorial 10: Adding wet deposition of chemical species**

## Tutorial 10

The current wet deposition scheme used by UKCA chemical tracers should be straightforward to add to.

Remember to keep track of array sizes.

# **Tutorial 11:**

# **Adding new UKCA chemical diagnostics**

## Tutorial 11

While the STASH system provides a nice GUI system for requesting output, it does introduce complexity within the code (and in the user-STASHmaster file format)

UKCA has a diagnostic system which deals with the STASH-handling, meaning that it is straight-forward to add-in new diagnostic requests

The code which deals with the diagnostics is in **`asad_chem_flux_diags.F90`**

You should not need to edit this module unless you want to make a new type of diagnostic

The specification of the diagnostics is done in the **`asad_flux_dat.F90`** module

# Tutorial 11

Currently UKCA can output the following types of diagnostics

- The flux through, or rate of, chemical reactions
- The flux through deposition processes
- The net chemical and dynamical tendencies of tracers
- The atmospheric mass
- PSC diagnostic information
- A dynamic 'tropospheric mask', useful for post-processing
- Tracer concentrations (which can be masked to only include tropospheric values)

Most diagnostics have units of moles/s

## Tutorial 11

To add new diagnostics you will need to

1. Define your diagnostic request in the `asad_flux_dat.F90` module

You will need to be careful here due to multiple possibilities from different chemistry schemes

2. Edit the STASHmaster\_A file to include this diagnostic
3. Request this diagnostic in the STASH panel

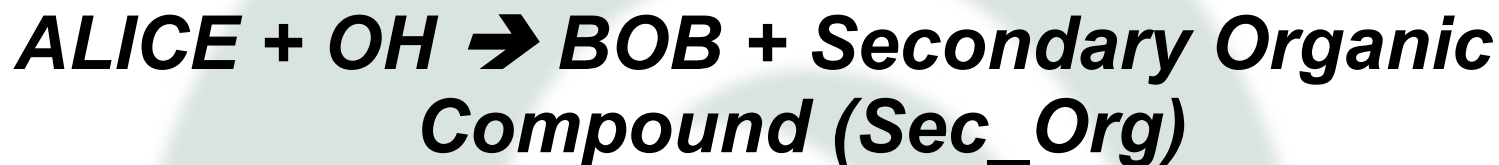
You can also use this diagnostic system to sum diagnostics on-line

- Multiple diagnostics sent to the same STASH code in `asad_flux_dat.F90` will be summed

## Tutorial 11

In this tutorial you are asked to

1. output the flux through the



reaction

2. Output the dry deposition of ALICE

3. Output the wet deposition of BOB

These should be daily means to the `pa/UPA` output stream.

**You should now work through the**

**11) Adding new UKCA chemical  
diagnostics**

**tutorial**



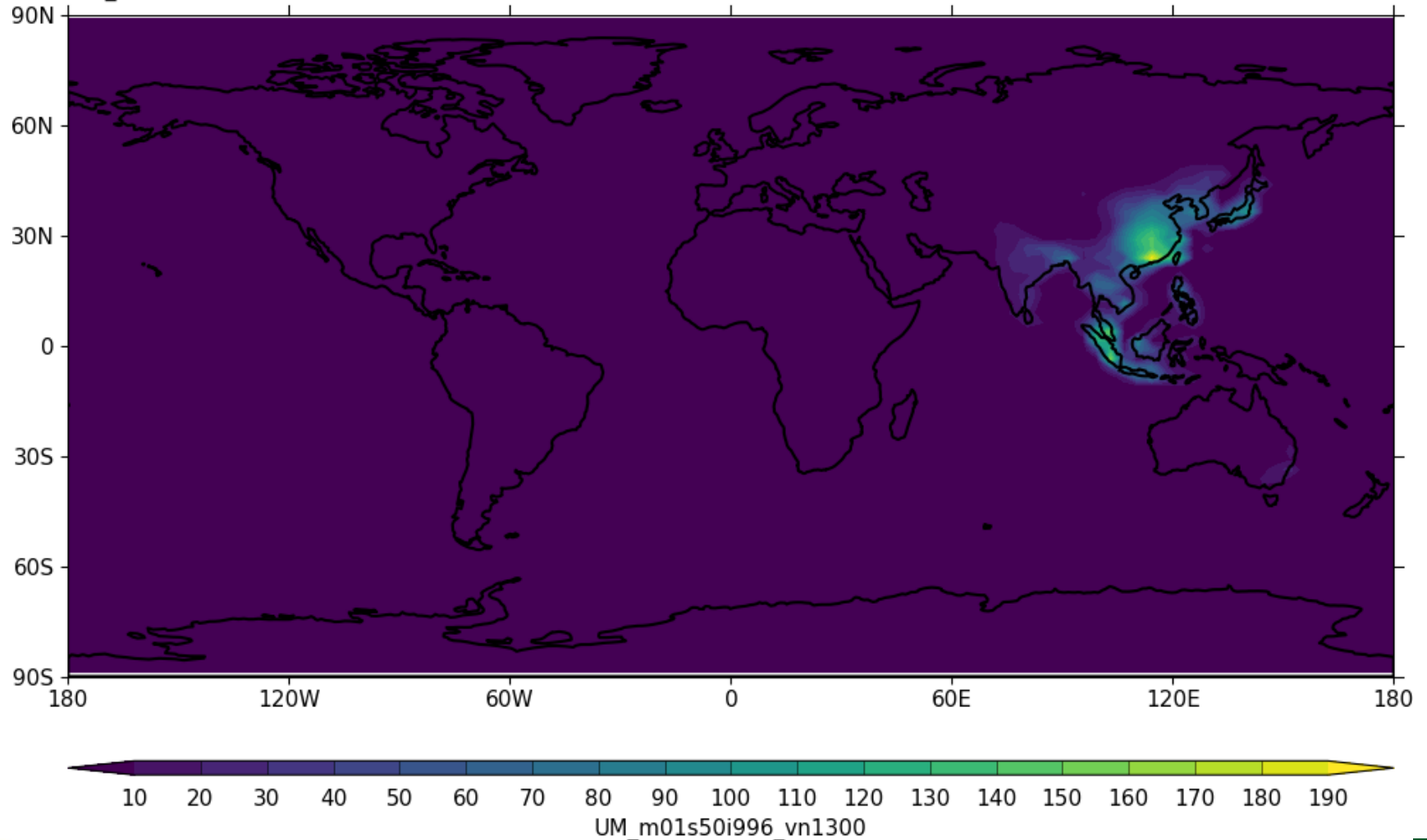


# **Tutorial 11: Adding new UKCA chemical diagnostics**

# Tutorial 11

ALICE+OH -> BOB+ Sec\_Org

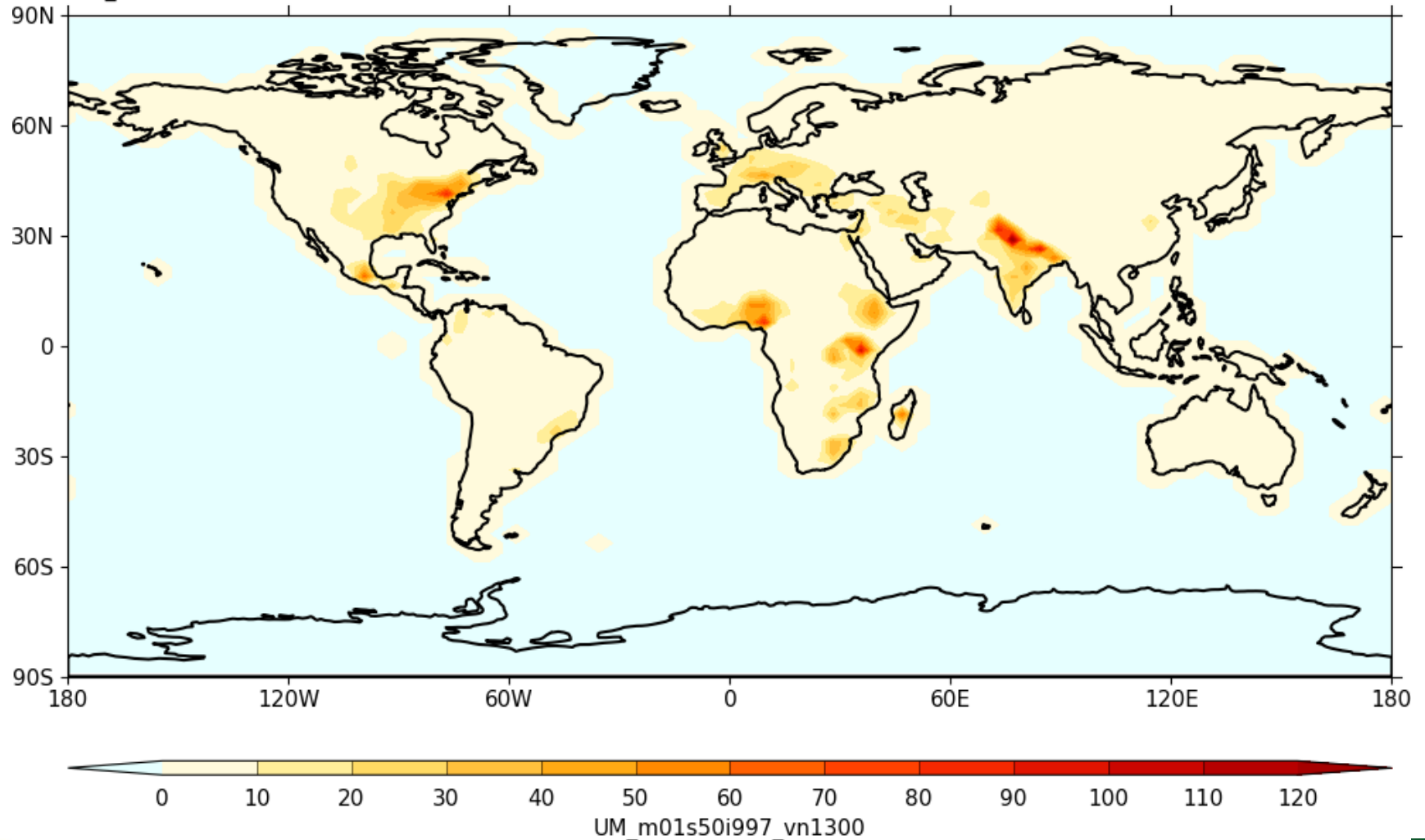
X: longitude (degrees\_east)  
Y: latitude (degrees\_north)  
Z: atmosphere\_hybrid\_height\_coordinate [0.0004714]  
cell\_methods: time: mean



# Tutorial 11

## ALICE surface dry deposition flux

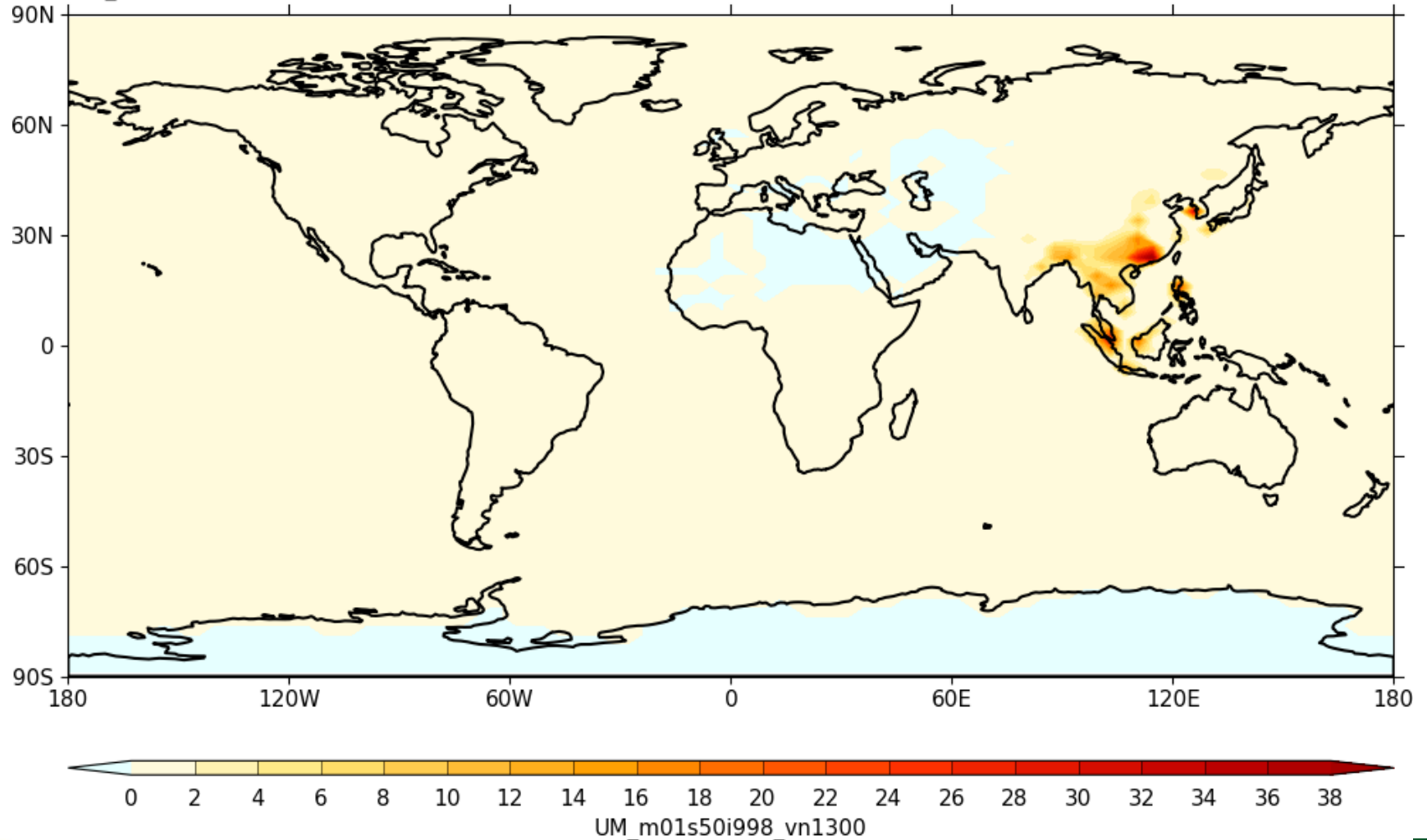
X: longitude (degrees\_east)  
Y: latitude (degrees\_north)  
Z: atmosphere\_hybrid\_height\_coordinate [0.0004714]  
cell\_methods: time: mean



# Tutorial 11

## BOB surface wet deposition flux

X: longitude (degrees\_east)  
Y: latitude (degrees\_north)  
Z: atmosphere\_hybrid\_height\_coordinate [0.0004714]  
cell\_methods: time: mean



## Points to remember

1. Be careful which STASH numbers you choose
  - The UKCA diagnostics are configured to sum multiple diagnostics to a single STASH number if defined this way
2. Be careful when implementing the different options dependent on chemistry scheme version, chemical mechanism used, whether aerosol chemistry is included etc.

# **Tutorial 12: Examining Aerosol Impacts**

## Tutorial 12

In this tutorial you are asked to

1. output various radiation (and aerosol diagnostics) to **pa/UPA** output stream on radiation timesteps
2. Make new time and domain profiles in STASH
3. Post-process these diagnostics
4. Alter the experimental set-up and assess the impact of not forming Sec\_Org, i.e. the reaction now becomes



**You should now work through the**

**12) Examining Aerosol Impacts**

**tutorial**





# **Tutorial 12: Examining Aerosol Impacts**

## Points to remember

1. STASH changes can be tricky, so take your time.
2. The cf-python and Iris python libraries can be used to read and process UM data
  - Take a look through the example scripts provided
  - How does cf-python compare to Iris?

# **Tutorial 13:**

# **Viewing and processing UKCA data with**

# **Python**

## Tutorial 13

In this tutorial you are asked to process and plot UKCA model output as well as an observational dataset.

1. UKCA pp-file output from an N96eL85 nudged simulation
2. Processed UKESM1 output in NetCDF format
3. Processed N48L60 UM-UKCA output in NetCDF format
4. The Bodeker total column ozone dataset

## Tutorial 13

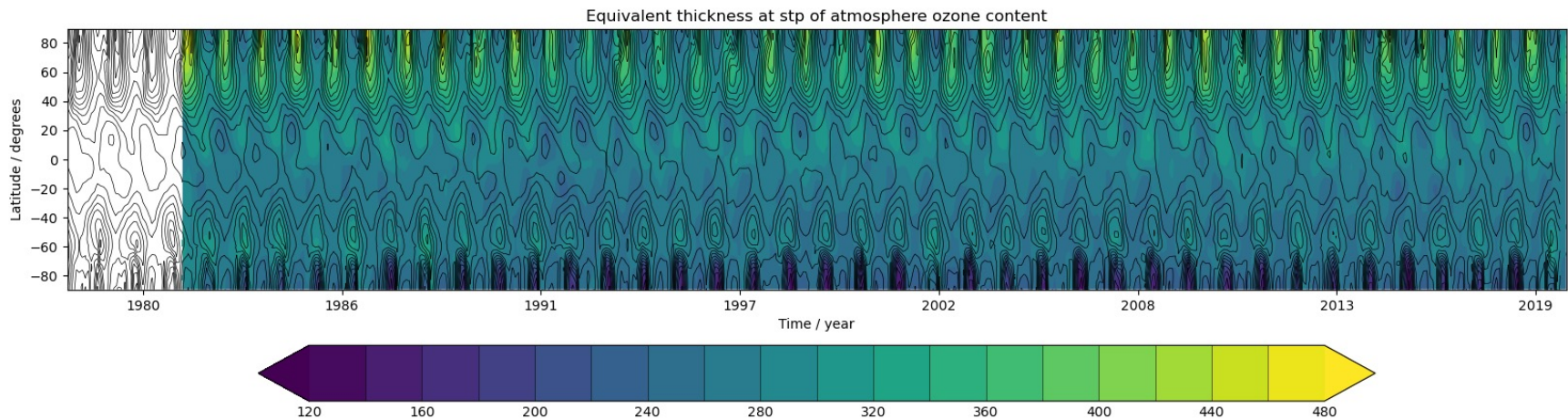
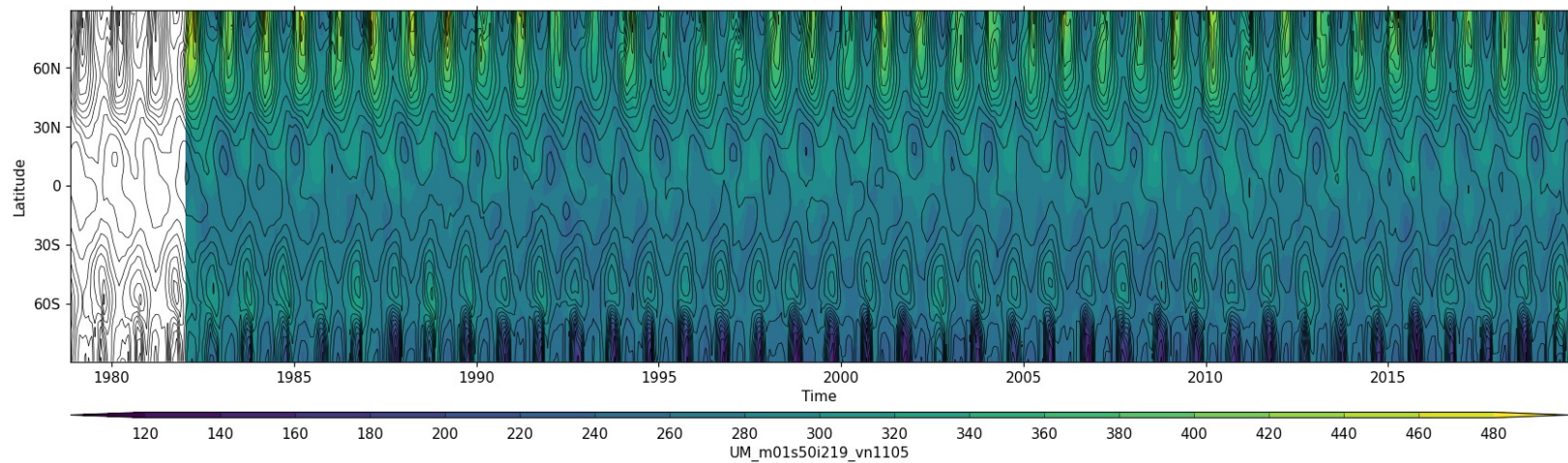
There is a mixture of resolutions and file formats for the 2D total column ozone data.

Examples are provided using both cf-python and the Iris Python libraries.

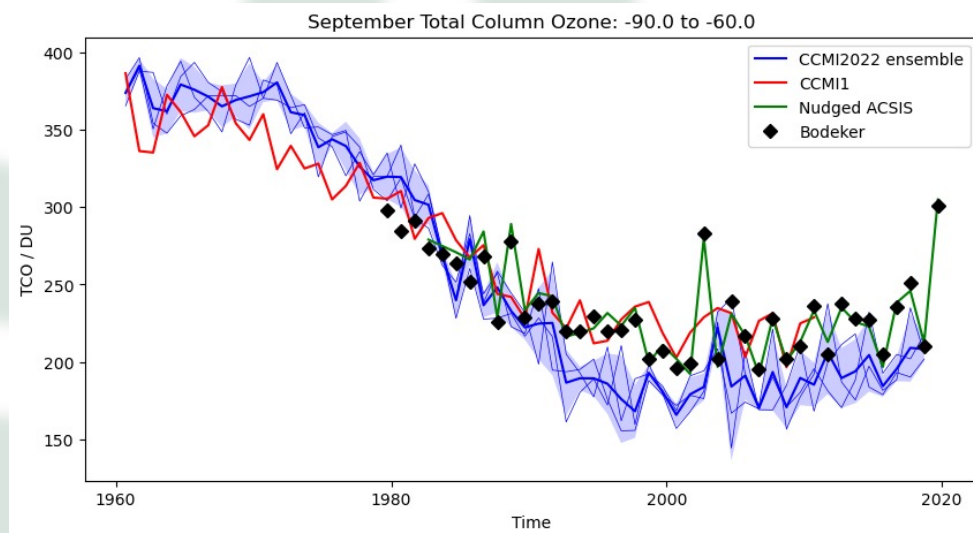
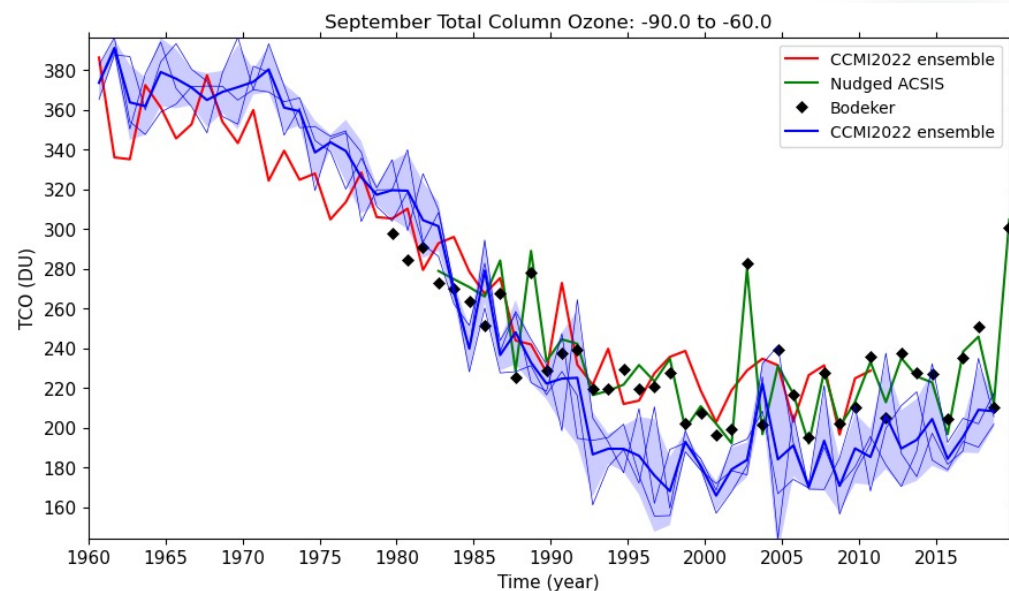
You should work through both sets of methods and compare them. At the end of each notebook are some exercises for you to try.



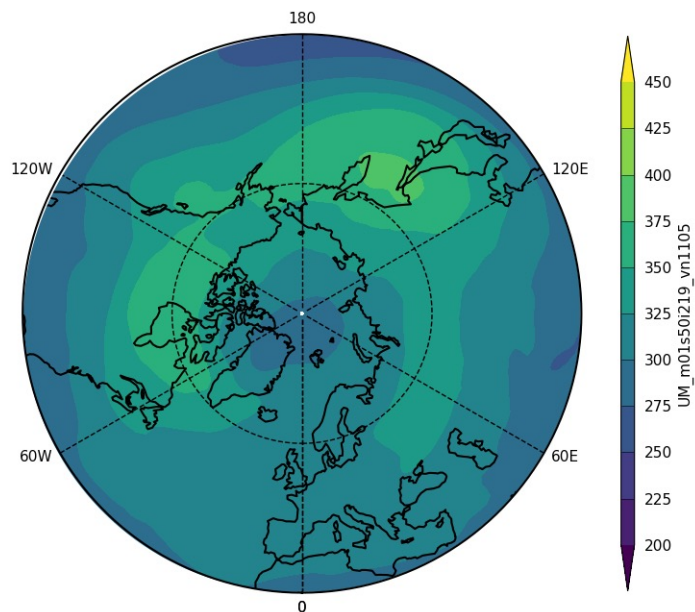
# Tutorial 13



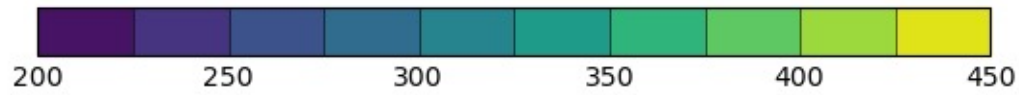
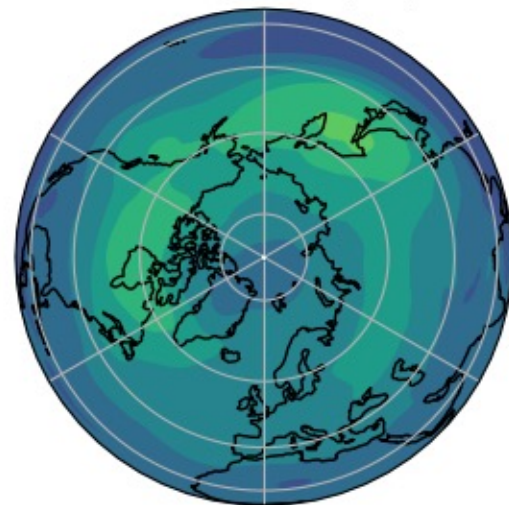
# Tutorial 13



# Tutorial 13

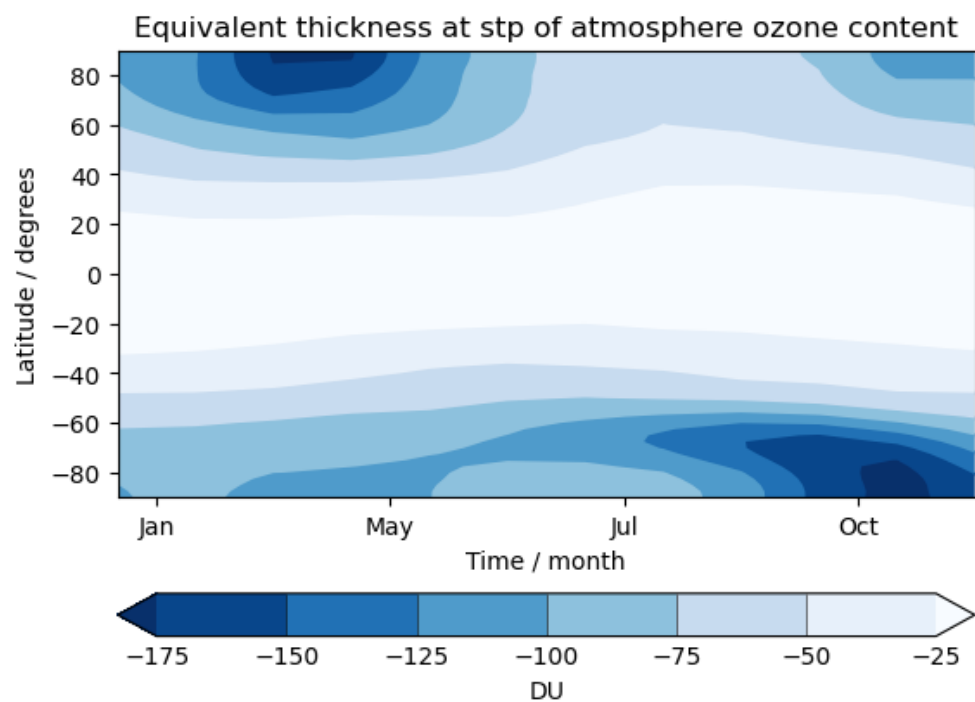
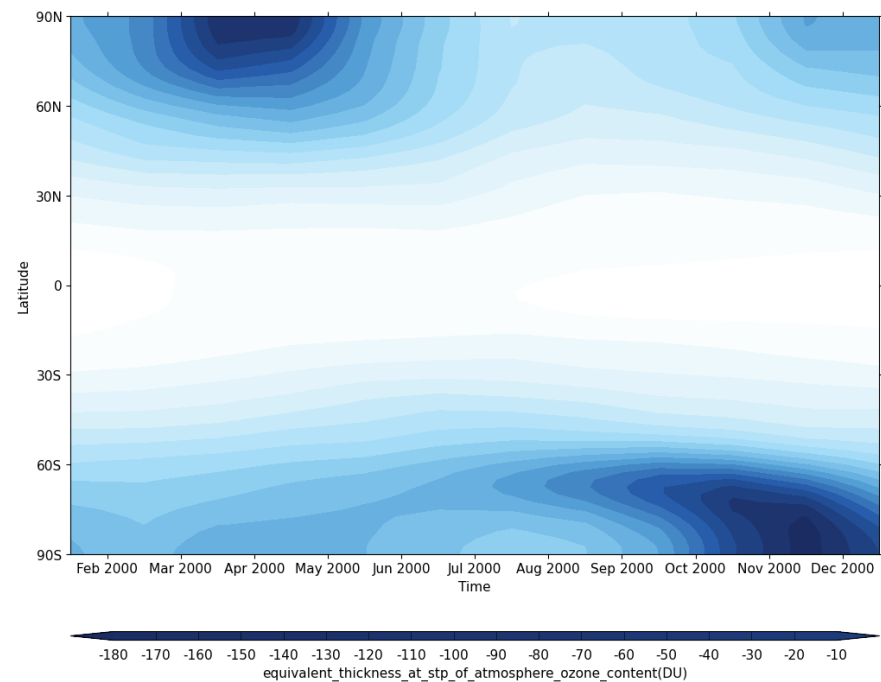


UKCA Total Column Ozone (DU) March 2011





# Tutorial 13



**You should now work through the**

**13) Viewing and processing UKCA data  
with Python**

**tutorial**



# **Tutorial 13: Viewing and processing UKCA data with Python**

### Points to remember

1. Both cf-python and Iris store the data in structures, known as Fields and Cubes respectively.
2. While some operations are similar, others are quite different – for example, the cf collapse function can calculate climatologies whereas this is done using the aggregated\_by function in Iris.
3. cf-python is often faster to read-in the data, especially for large datasets, but Iris may be quicker at performing some other operations.
4. It is not possible to mix-and-match between the libraries, you can only use one at a time.

# What should you now be able to do with UKCA?

After doing these Tutorials you should

- Be more confident using Rose

- Be able to copy existing UKCA suites, run them, and be able to view and process the output

- Be able to add new UKCA tracers

- Be able to define new and edit existing chemical reactions

- Be familiar with STASH and working with UM output

- Be able to create and add emissions into UKCA

- Be able to define new dry and wet deposition of chemical species

- Be able to output new chemical diagnostics



## Feedback

I hope that you will find the UKCA Tutorials both enjoyable and useful.

It would be very helpful for me if you could complete the UKCA Tutorials feedback form, and more detailed comments can be emailed to me at

**`n.luke.abraham@ncas.ac.uk`**

Any and all feedback given will be used to improve the Tutorials for future users.

## Next Steps with UKCA

- The UM (& UKCA) is available for UK academic users on ARCHER2, and for those with a collaboration with the Met Office, on Monsoon2
- The Met Office have also enabled running the UM in a Virtual Machine environment.
  - This means that you can develop code and test configurations on your own desktop, without requiring a supercomputer
  - You have been using this environment for this training

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

Geosci. Model Dev., 11, 3647–3657, 2018

<https://doi.org/10.5194/gmd-11-3647-2018>

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## **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**

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**<https://www.geosci-model-dev.net/11/3647/2018/>**