UNIVERSITY OF CAMBRIDGE

Introduction to UKCA

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Centre *for* **Atmospheric Science**

Outline

What is UKCA and what can I do with it?

Practicals

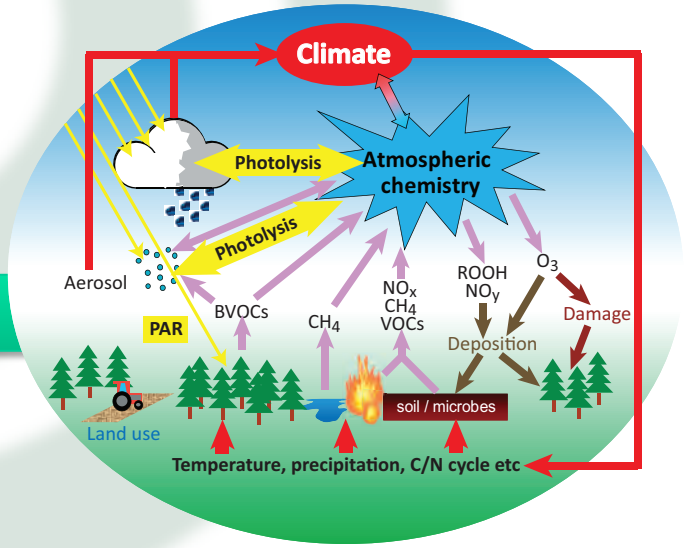
Next Steps

What is UKCA?

UKCA is a Climate-Chemistry-Aerosol model, built as a sub-model of the Met Office's Unified Model (UM).

UKCA is not a *particular* collection of chemistry and aerosol schemes, but is a **framework** for putting chemistry and aerosol schemes into the UM.

Unified Model



UKCA

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, covering the troposphere and the stratosphere

- These schemes are 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 Practicals is to teach new UKCA users how to do this

Practicals

The course will take place here in the G30 computer room, near the main entrance to the Department.

Tea/Coffee will be in the BMS Lecture Theatre from 11am and 3pm. Lunch will be in the BMS from 12.30pm.

Note that food and drink is not allowed in G30.

Practicals

- The Practicals make use of GA7.0 and the Rose/Cylc interface at UM vn10.9.
- There are a number of differences between these and the previous versions of the practicals.
- The Tutorial jobs are a cut-down configuration designed for training and testing.

Using UKCA

- What resources are available?
  - UKCA Evaluation Suite
  - NCAS Computational Modelling Services
  - Met Office Science Repository Service

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, ARCHER, & JASMIN

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
- UKCA jobs output a set of standard diagnostics which are then read by the suite to produce a series of plots to aid model evaluation
- This suite is also designed to inform the UKCA developers whether or not a candidate job is scientifically suitable for release
- ARCHER: **`/work/n02/n02/ukca/Eval`**

UKCA Evaluation Suite

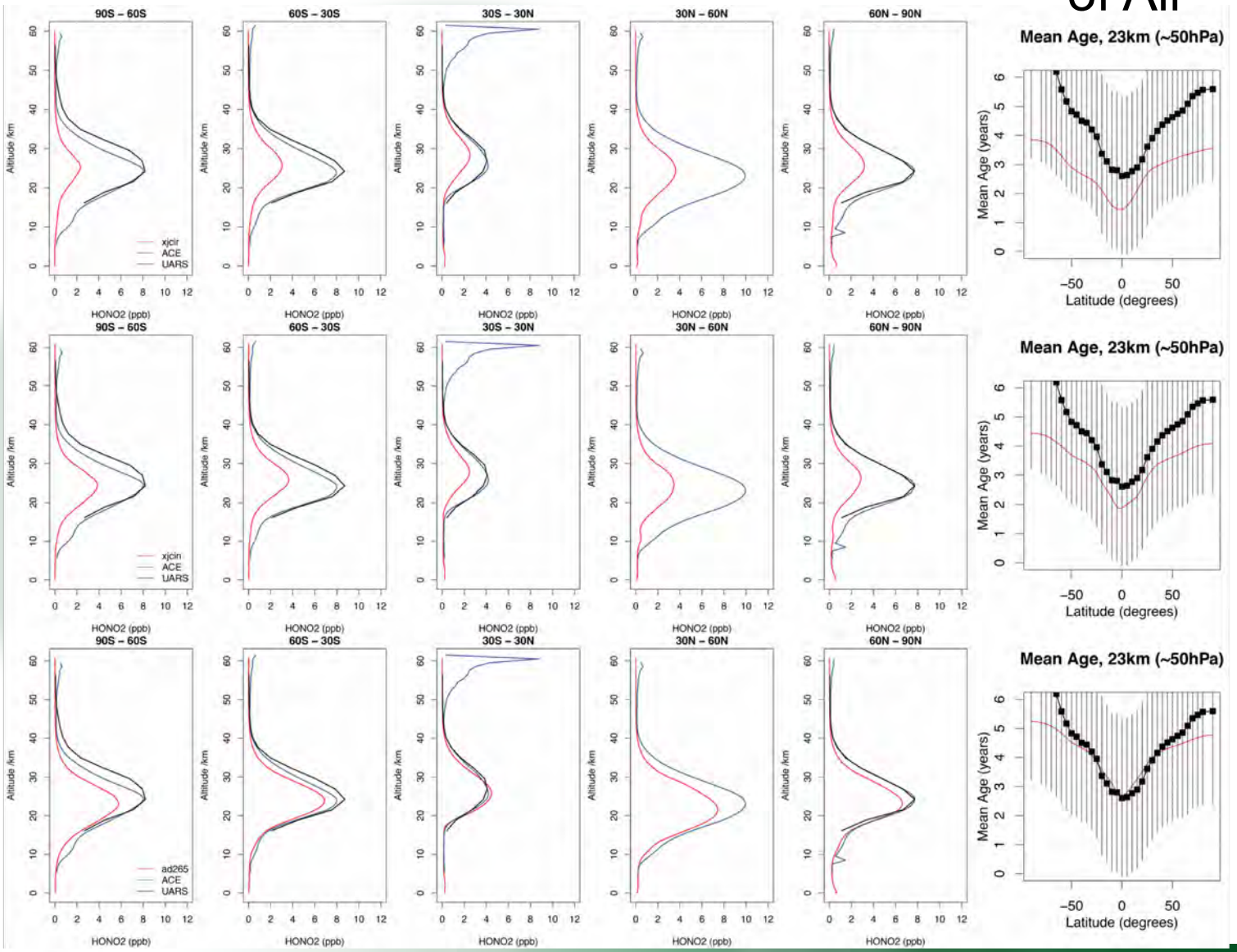
NOy

Age of Air

vn7.3
HadGEM3-A
r2.0 N48L60

vn8.4
GA4.0

vn10.3
GA7.0



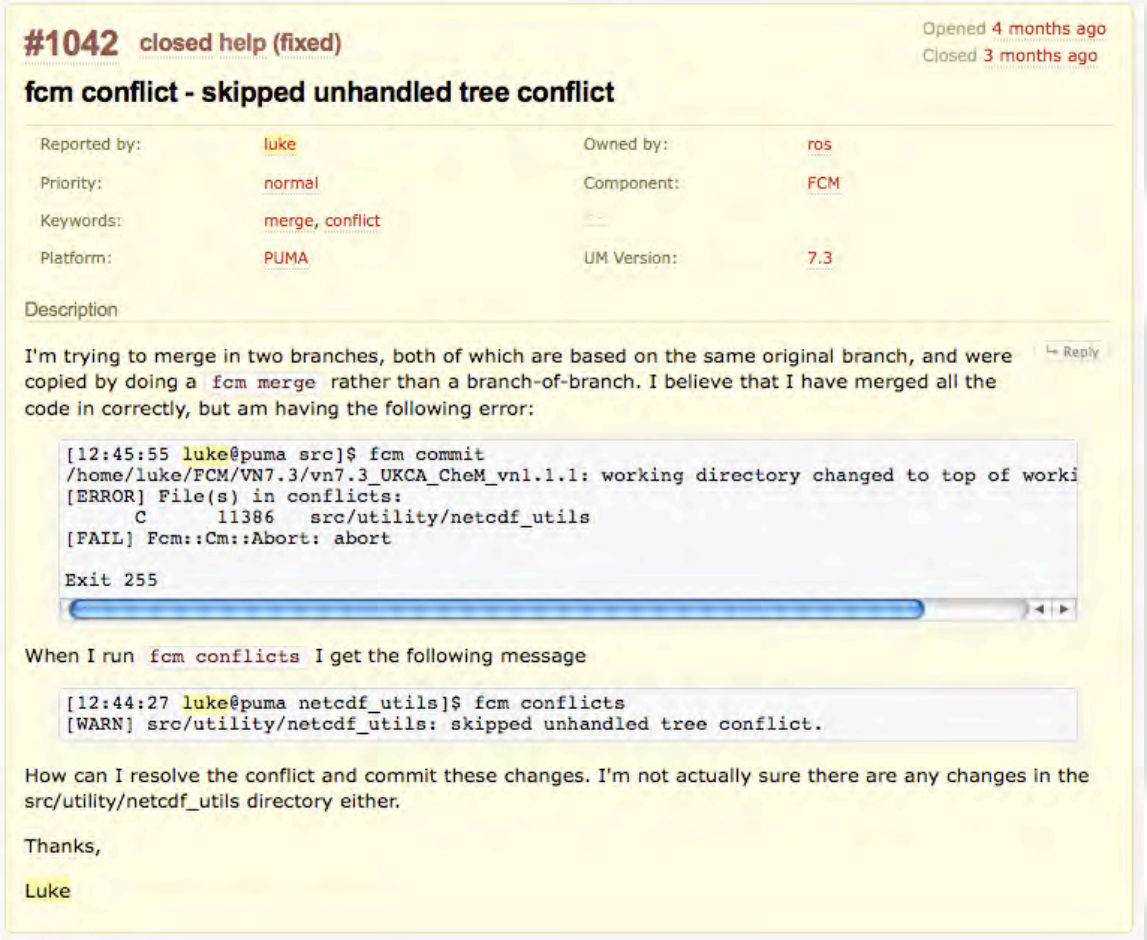
What do CMS do?

- CMS provide the PUMA service. This runs the UMUI & Rose/Cylc servers which is used to submit UM jobs to ARCHER and MONSooN (UMUI only)
- 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, and the cf-python library
- They manage the NERC atmospheric group on ARCHER (`n02`)
- They provide the **CMS Helpdesk**

Helpdesk

Ticket	Summary	Component	Version	Type	Owner	Status	Created
#1105	Segmentation fault when using the PC2 cloud scheme	UM Model	6.6.3	help	willie	accepted	24/07/13
#1104	UM4.5.1 on HECToR (July 2013)	UM Model	4.5	help	um_support	new	19/07/13
#1103	Error in umui	UMUI	<select version>	help	um_support	new	19/07/13
#1101	PS31 MOGREPS on MONSooN	UM Model	8.2	enhancement	willie	new	12/07/13
#1100	MOGREPS-R data request	Data	<select version>	task	um_support	new	12/07/13
#1098	large drift in HadGEM2 concides with change to phase2b..	UM Model	6.6.3	help	ros	accepted	10/07/13
#1097	Sending files straight to local computer	UM Model	None	help	ros	new	10/07/13
#1095	Running the UM with SST anomalies	UM Model	7.3	help	willie	accepted	08/07/13
#1092	Radiation diagnostics on different timestep to other variables?	UM Model	6.6.3	help	um_support	new	27/06/13
#1091	problems using sea ice and sst ancillaries	UM Model	6.6.3	help	jeff	accepted	27/06/13
#1088	PS31 Euro4 on MONSooN	UM Model	8.2	help	willie	new	21/06/13
#1087	Ensembles on MONSooN	UM Model	8.2	help	willie	new	21/06/13
#1081	Unknown problem in .leave file when submitting job	UM Model	6.6.3	help	um_support	new	11/06/13
#1071	UKCA O3-NOy daily output run failed	UM Model	7.3	help	luke	accepted	20/05/13
#1070	running HadCEM at Bristol	UM Model	4.5	help	jeff	new	16/05/13
#1067	Failure of model run using IAU scheme - segmentation fault	UM Model	6.6.3	help	um_support	assigned	13/05/13
#1064	Sporadic problems submitting to MONSOON (error msg: "system has no more ptys"	UM Model	7.3	help	um_support	new	07/05/13
#1061	segmentation fault when running HadCEM	UM Model	4.5	error	um_support	new	03/05/13
#1059	ssh_exchange_identification: Connection closed by remote host	UM Model	<select version>	help	um_support	new	01/05/13
#1053	Model instability	UM Model	7.3	help	luke	accepted	15/04/13
#1051	UKCA NOy stash diagnostics&NOx emissions	UM Model	7.3	help	luke	accepted	10/04/13
#1035	xancil - error	UM Model	6.1	help	jeff	accepted	08/03/13
#988	Network timeout submitting jobs to MONSooN	MONSooN	7.3	error	ros	reopened	06/12/12
#981	Sea ice ancillary file causing model crash	UM Model	7.3	help	jeff	accepted	03/12/12
#892	Error when reconfiguring a minimal start dump without physics	UM Model	8.2	help	annette	reopened	16/08/12
#769	Error when attempting to run an ensemble	UM Model	7.8	error	simon	assigned	10/01/12
#648	UM version 4.5.3 (FAMOUS) compilation problem	FAMOUS	4.5	error	robin	accepted	11/07/11
#583	12-hour and 6-hour means	UMUI	<select version>	help	lois	assigned	16/02/11

Helpdesk



#1042 closed help (fixed)

Opened 4 months ago
Closed 3 months ago

fcm conflict - skipped unhandled tree conflict

Reported by:	luke	Owned by:	ros
Priority:	normal	Component:	FCM
Keywords:	merge, conflict		
Platform:	PUMA	UM Version:	7.3

Description

Reply

I'm trying to merge in two branches, both of which are based on the same original branch, and were copied by doing a `fcm merge` rather than a branch-of-branch. I believe that I have merged all the code in correctly, but am having the following error:

```
[12:45:55 luke@puma src]$ fcm commit
/home/luke/FCM/VN7.3/vn7.3_UKCA_CheM_vn1.1.1: working directory changed to top of worki
[ERROR] File(s) in conflicts:
      C      11386   src/utility/netcdf_utils
[FAIL] Fcm::Cm::Abort: abort

Exit 255
```

When I run `fcm conflicts` I get the following message

```
[12:44:27 luke@puma netcdf_utils]$ fcm conflicts
[WARN] src/utility/netcdf_utils: skipped unhandled tree conflict.
```

How can I resolve the conflict and commit these changes. I'm not actually sure there are any changes in the src/utility/netcdf_utils directory either.

Thanks,

Luke

Solved in 5 comments

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.

UKCA tickets will be answered by Luke Abraham.

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

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

ALICE + OH ➔ BOB + Secondary Organic Compound (Sec_Org)

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
  - Rose changes
    - Editing of STASHmaster_A (diagnostic definition) file & associated metadata changes
    - Changes to STASH (diagnostic) output
  - UKCA code changes
    - New species
    - New emissions
    - New reactions/depositions
    - Changing the aerosol configuration
  - Working with various UM files
    - Regridding input data
    - Creating netCDF files
    - Processing UM output

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 several tutorials

2. Remember that UKCA sits within the UM framework

Tutorial Tasks

The Tutorials are broken down into three sections

1. General use of UKCA and Rose

   These three tutorials cover the basics of the copying and running a UKCA suite, before outputting a field through STASH

2. UKCA Chemistry

   These tutorials break down the chemistry task into 6 smaller chunks

   - Adding tracers, adding emissions, adding reactions, adding dry and wet deposition, and adding chemical diagnostics

3. UKCA Aerosols

   The aerosol tutorial covers looking at the aerosol optical depth and other quantities in more detail.

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.

Feedback

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

It would be very helpful for me if you could fill in the UKCA feedback form which will be sent to you.

More detailed comments can be emailed to me at

`luke.abraham@atm.ch.cam.ac.uk`

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

The Tutorials

Tutorial 1:
Running an existing UKCA suite

Tutorial 1: Running an existing UKCA suite

This tutorial is designed to make you more familiar with the use of Xconv to view UKCA output

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

ARCHER: **u-as101**

Tutorial 1: Running an existing UKCA suite

- During the practical sessions we will be making use of a reserved queue on ARCHER
  - This is tied to your training account **`ncastrXX`**
  - To ensure that you are running in this queue you need to make sure that you select the correct queue to run on (e.g. *'Tuesday 8th Jan 2019'*). **This will need to be changed every day.**
- You will also need to first make sure that your SSH-key has been copied across to your ARCHER training account, and that you have set-up your .profile correctly

`http://cms.ncas.ac.uk/documents/training/December2017/UM_practicals/getting-setup.html`

Tutorial 2:
Exploring Rose

Tutorial 2: Exploring Rose

- This tutorial is designed to make you more familiar with Rose
- Rose is the UM *namelist* editor, which also provides some consistency checking on the choices made.
- There is help text for each variable, and may have allowed ranges/values defined
- You should take a look through Rose while your suite is running. Don't worry about clicking on things – there is an **undo** button!

Tutorial 3:
STASH

Tutorial 3: STASH

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

You should now work through the

1) Running an existing UKCA suite
2) Exploring Rose
3) What is STASH?

tutorials

Tutorial 1:
Running an existing UKCA suite

Points to remember

1. You can check the progress of a running job by looking at the output in the **`atmos.fort6.pe00`** file
2. Warning and error messages are held in the output **`job.err`** file

Tutorial 2:
Exploring Rose

Points to remember

1. Rose is a namelist editor, with a search function, so it should be straight-forward to find the variable(s) of interest
2. Remember that there is help text available for each variable
3. If you are unsure what you are looking for, browse through the Rose panels, view the information on each variable to see what options are available
4. Remember that there is an ‘undo’ button
5. You need to save the suite prior to being able to run it, but you should also ‘fcm commit’ the suite configuration (periodically) as well

Tutorial 3:
STASH

Tutorial 3: STASH

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 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 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 4:
Adding new UKCA tracers

Tutorial 4: Adding new UKCA tracers

This tutorial begins the process of adding in the new tracers, emission, reaction, depositions, and diagnostics

You are asked to add in two tracers, ALICE and BOB

Tutorial 5:
Adding new emissions

Tutorial 5: Adding new emissions

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
- 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 N96e resolution and then use this in UKCA

You should now work through the

4) Adding new chemical tracers
5) Adding new emissions

tutorials

Tutorial 4:
Adding new UKCA tracers

Tutorial 4: Adding new UKCA tracers

Points to remember for the Rose changes:

1. Pick your tracer slot(s) from the UKCA code
2. Edit the STASHmaster_A file for these, and add them to the Rose STASH panel
   - Remember to initialise the tracer as well as output it
   - Remember to define the pressure-level equivalent(s)

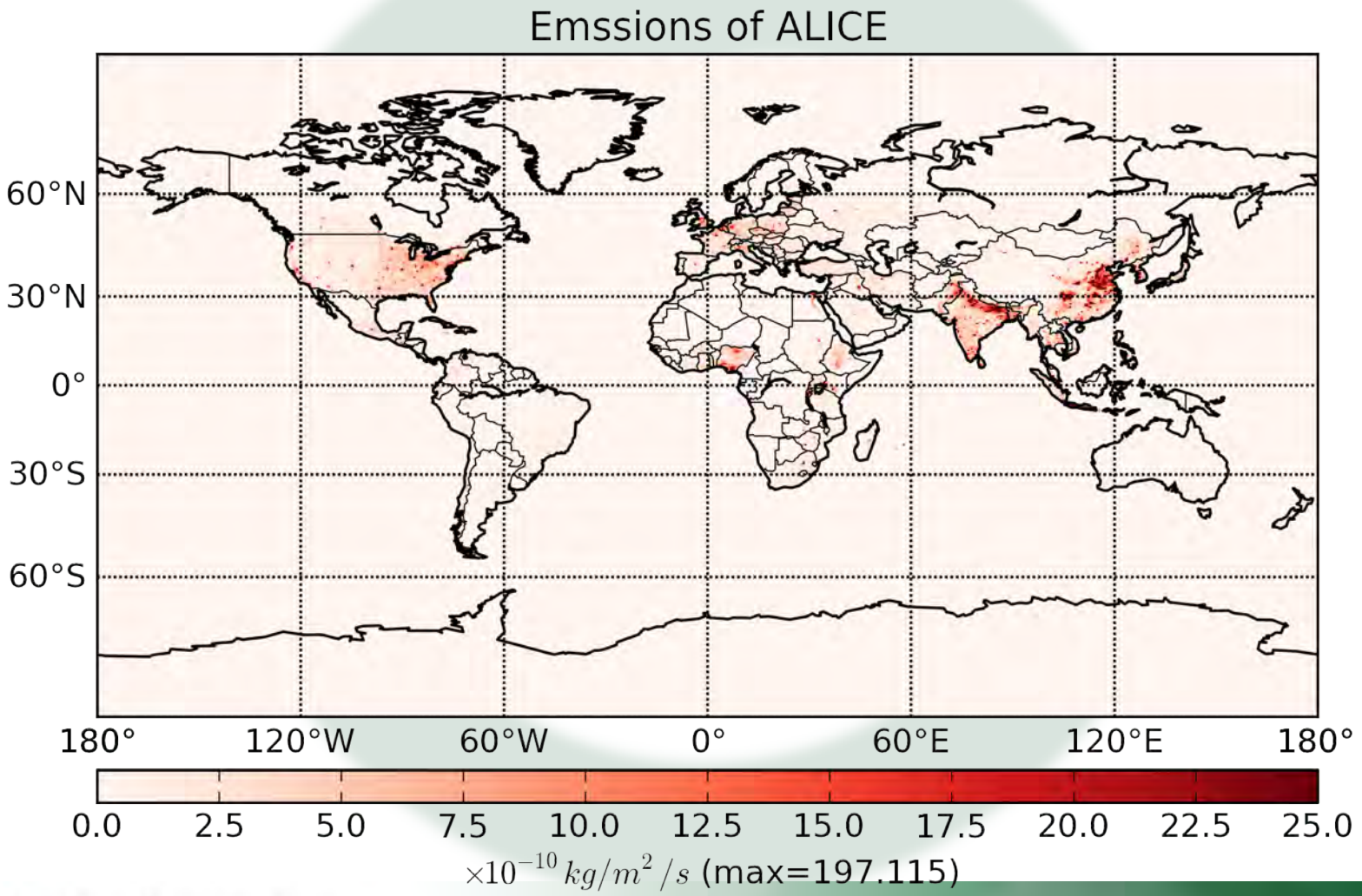
Once you have done these, you can make your UKCA changes

Points to remember for the UKCA 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 H2O 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, you will need to define a conversion factor for your new tracers

Tutorial 5:
Adding new emissions

Tutorial 5: Adding new emissions



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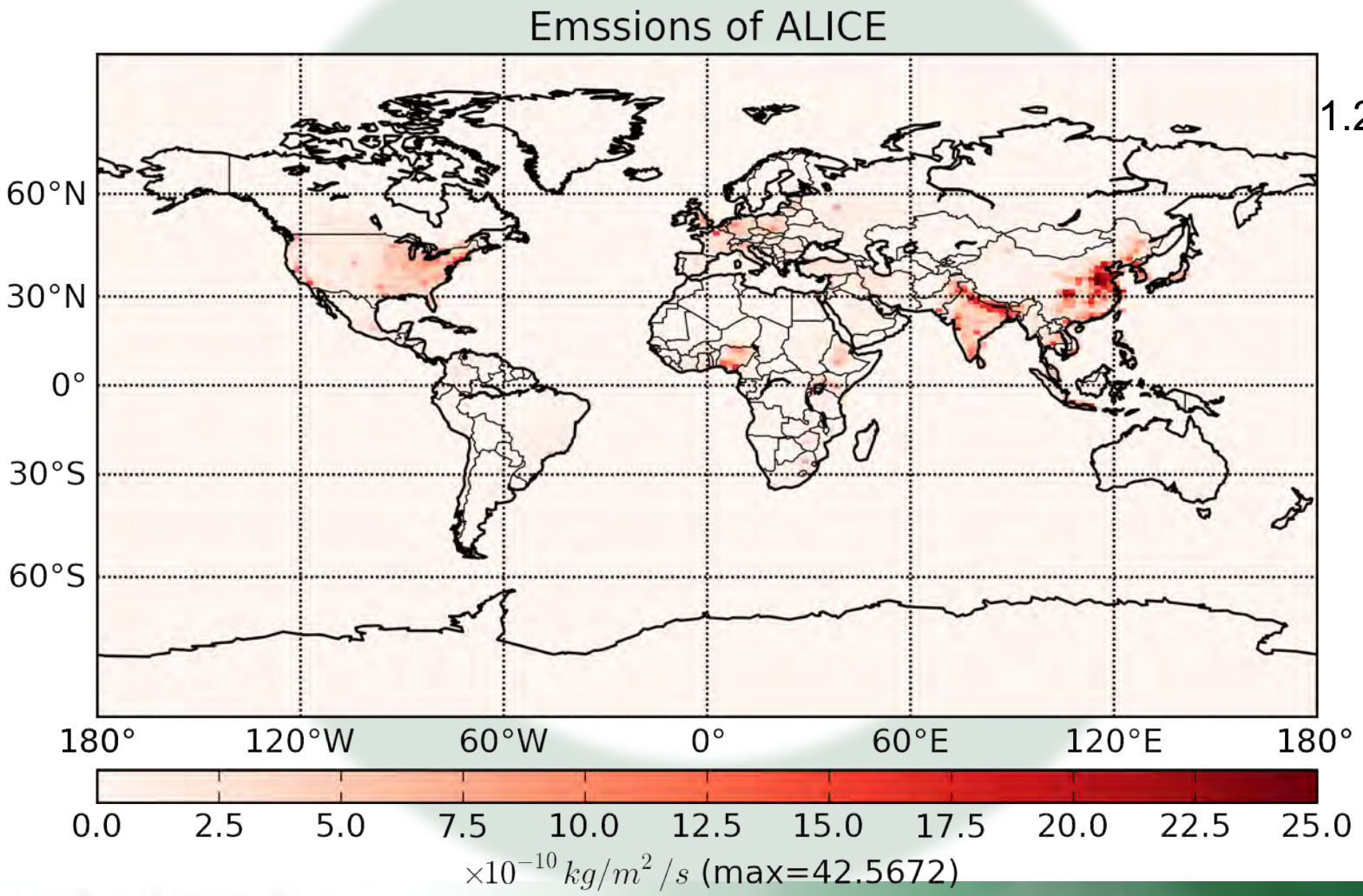
Tutorial 5: Adding new emissions



N96
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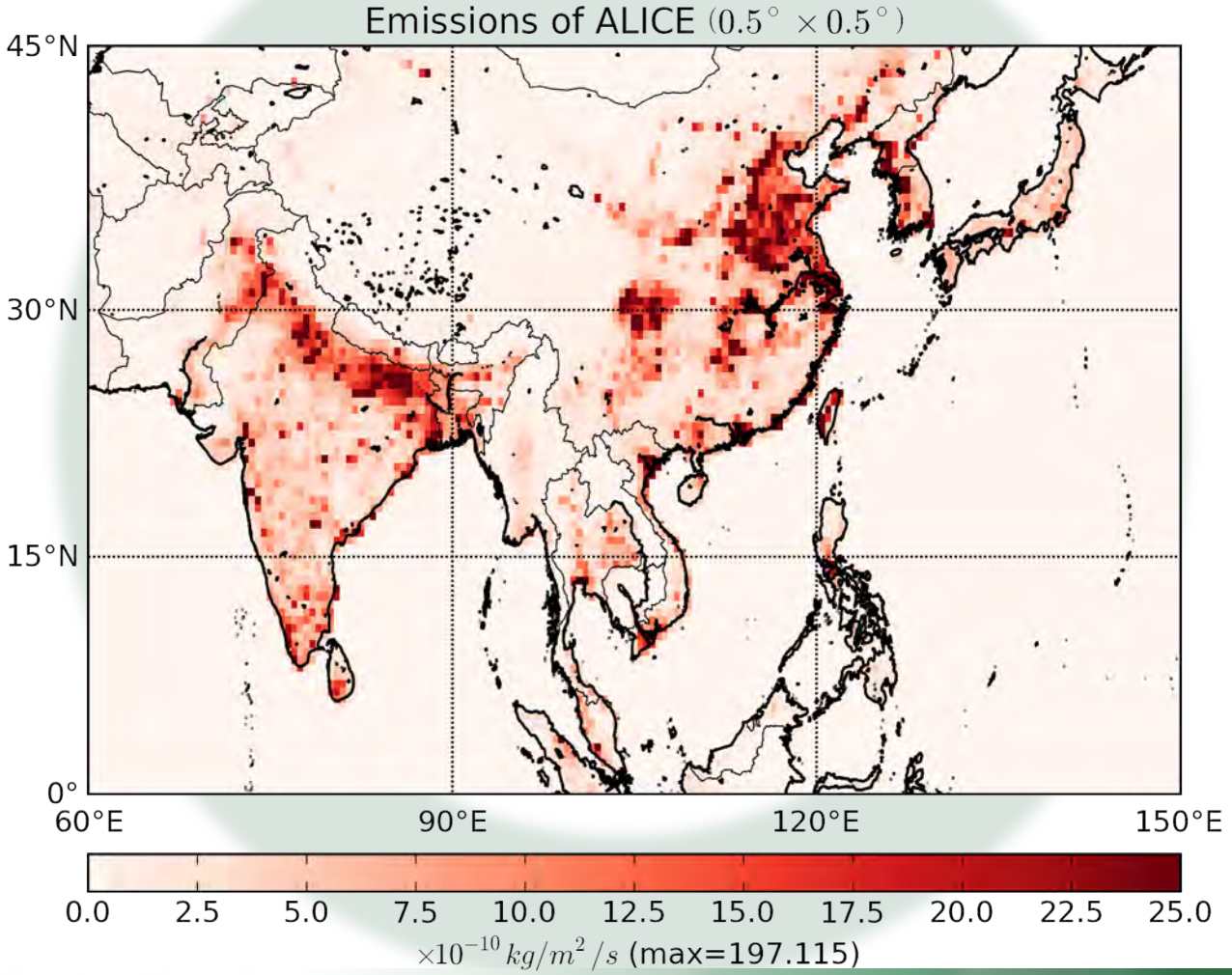
Tutorial 5: Adding new emissions



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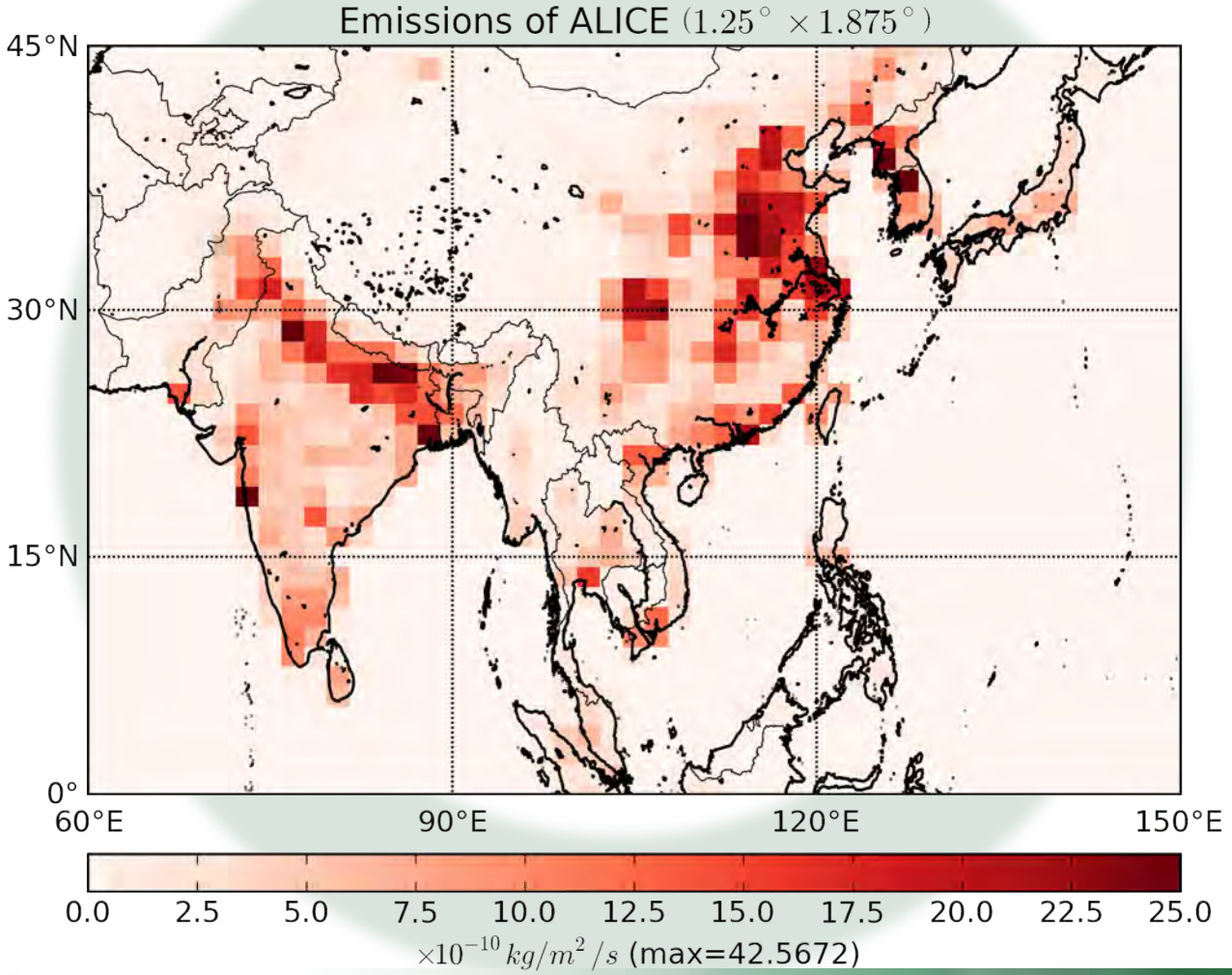
Tutorial 5: Adding new emissions



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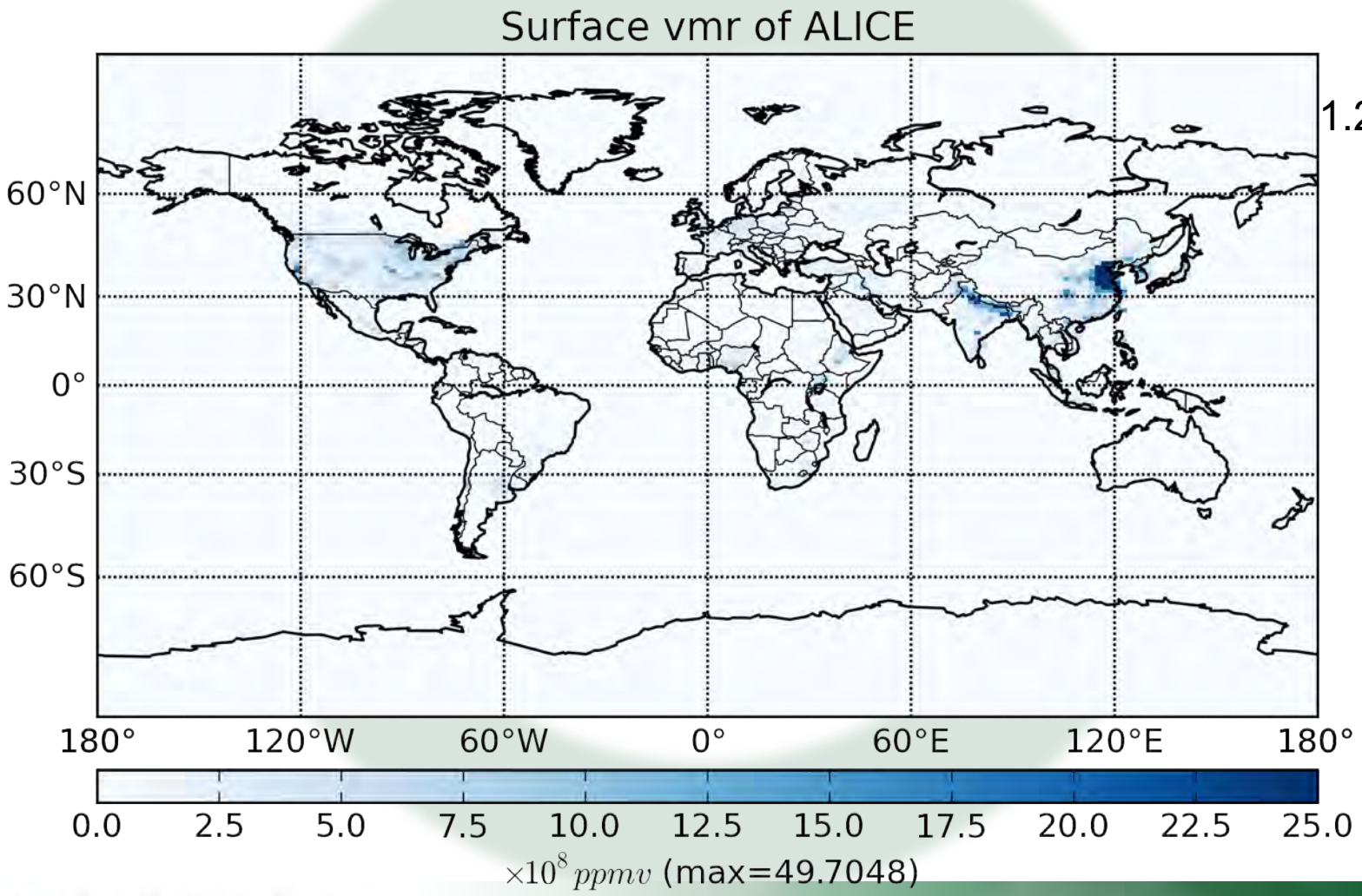
Tutorial 5: Adding new emissions



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Tutorial 5: Adding new emissions

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 6:
Adding new reactions

Tutorial 6: Adding new reactions

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 6: Adding new reactions

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

ALICE + OH ➔ BOB + Secondary Organic Compound (Sec_Org)

using the following rate coeffients

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

$$\alpha = 0.00$$

$$\beta = -390.0$$

You should:

Make your changes to the UKCA chemistry specification module

Tutorial 7:
Adding dry deposition

Tutorial 7: Adding dry deposition

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 7: Adding dry deposition

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

	Summer (day)	*Summer (night)*	*Summer (24h av)*	*Winter (day)*	*Winter (night)*	*Winter (24h av)*
Water	0.0	0.0	0.0	0.0	0.0	0.0
Forest	0.3	0.3	0.3	0.3	0.3	0.3
Grass	0.3	0.3	0.3	0.3	0.3	0.3
Desert	0.3	0.3	0.3	0.3	0.3	0.3
Ice	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_surfddr`**, taking the different molecular mass of ALICE into account

Tutorial 8:
Adding wet deposition

Tutorial 8: Adding wet deposition

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

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

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

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

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

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

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

Tutorial 9:
Adding new UKCA diagnostics

Tutorial 9: Adding new UKCA diagnostics

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`**
  - 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`** module

Tutorial 9: Adding new UKCA diagnostics

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 9: Adding new UKCA diagnostics

To add new diagnostics you will need to

1. Define your diagnostic request in the **`asad_flux_dat`** module
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`** will be summed (useful for budgeting)

Tutorial 9: Adding new UKCA diagnostics

In this tutorial you are asked to

1. output the flux through the

   ALICE + OH → BOB + Secondary Organic Compound (Sec_Org)

   reaction to STASH code 50134
2. Output the dry deposition of ALICE to STASH code 50135
3. Output the wet deposition of BOB to STASH code 50136

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

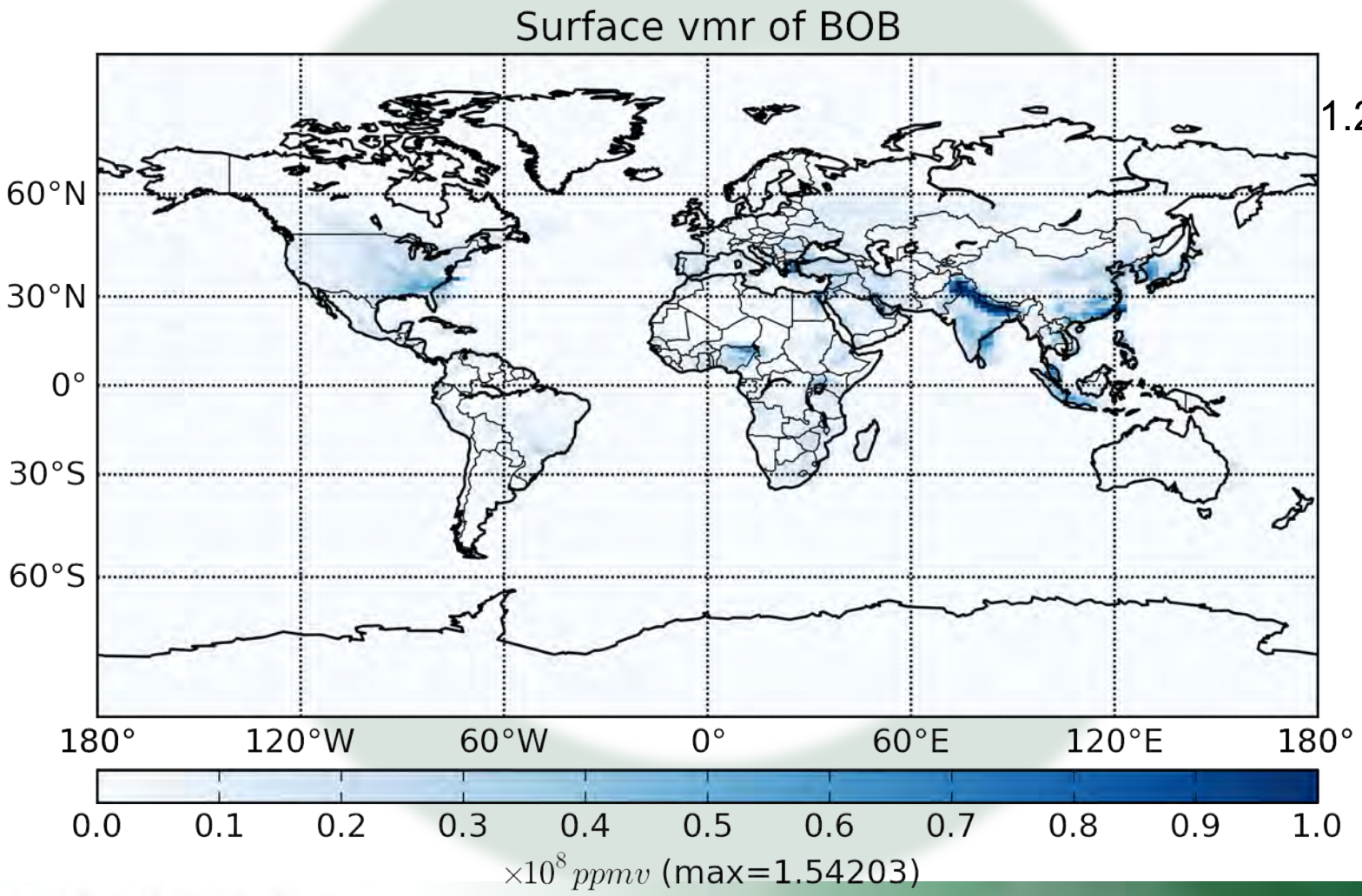
You should now work through the

6) Adding new chemical reactions
7) Adding dry deposition of chemical species
8) Adding wet deposition of chemical species
9) Adding new UKCA diagnostics

tutorials

Tutorial 6:
Adding new reactions

Tutorial 6: Adding new reactions



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Points to remember

1. Check that you have your array sizes correct – it can be difficult to keep track

Tutorial 7:
Adding dry deposition

Points to remember

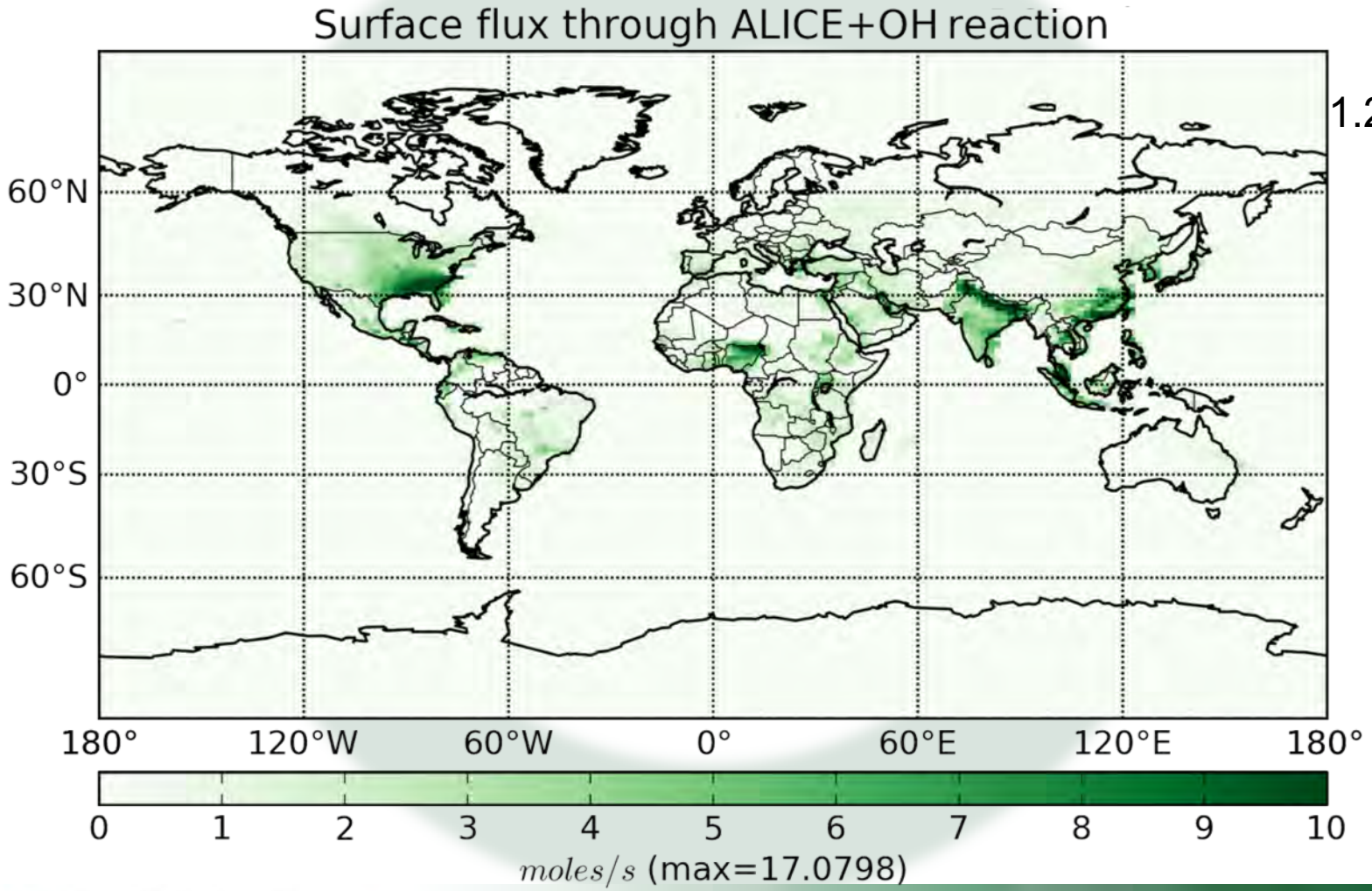
1. Even if you are using the Interactive scheme, you will also need to make changes to the 2D scheme
2. When adding species to the Interactive scheme you may also need to define the molar mass of the deposited species
   - Remember that there are options for 9, 13, 17, & 27 surface types

Tutorial 8:
Adding wet deposition

Tutorial 8: Adding wet deposition

Tutorial 9:
Adding new UKCA diagnostics

Tutorial 9: Adding new UKCA diagnostics



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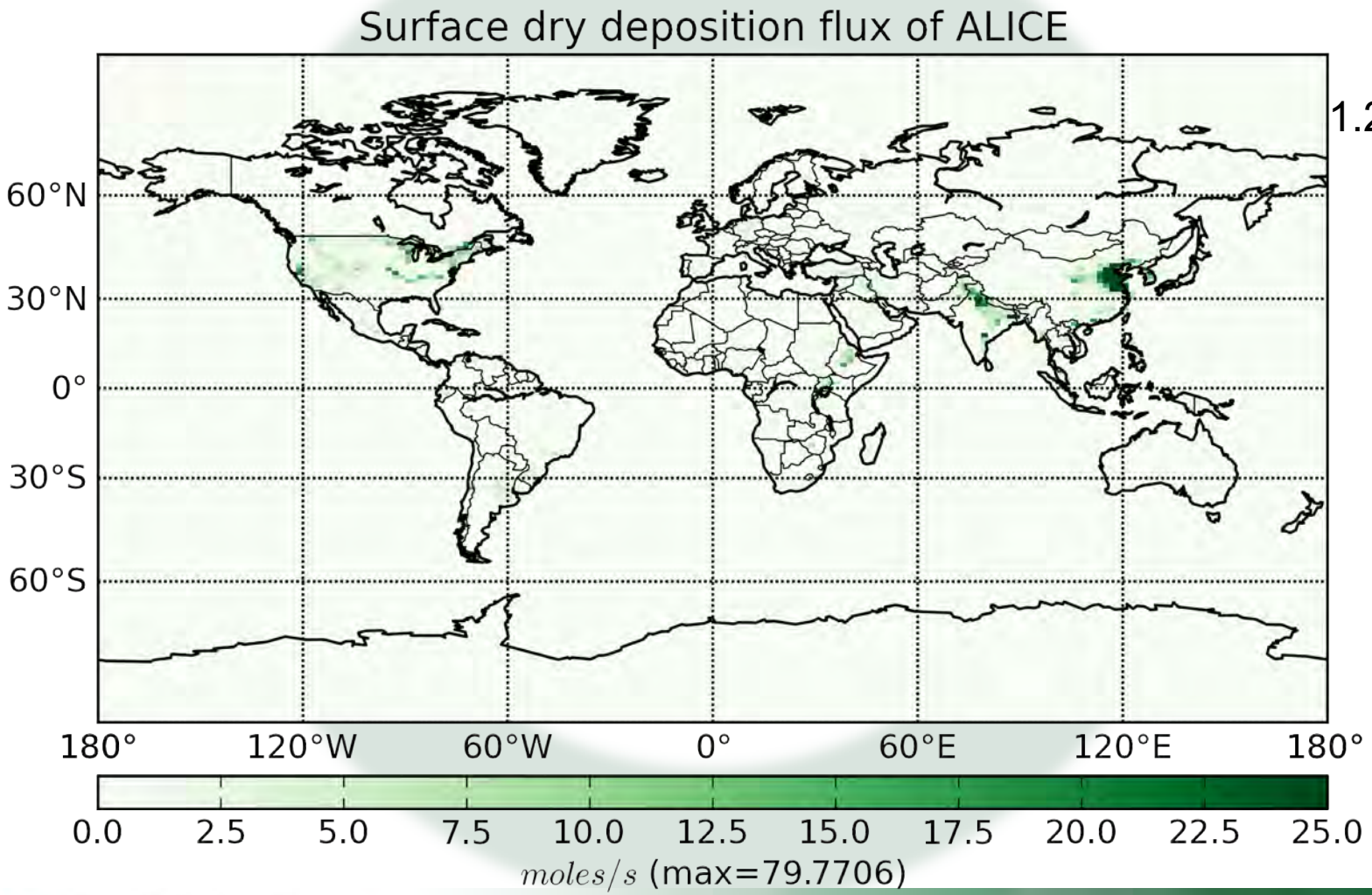
Tutorial 9: Adding new UKCA diagnostics



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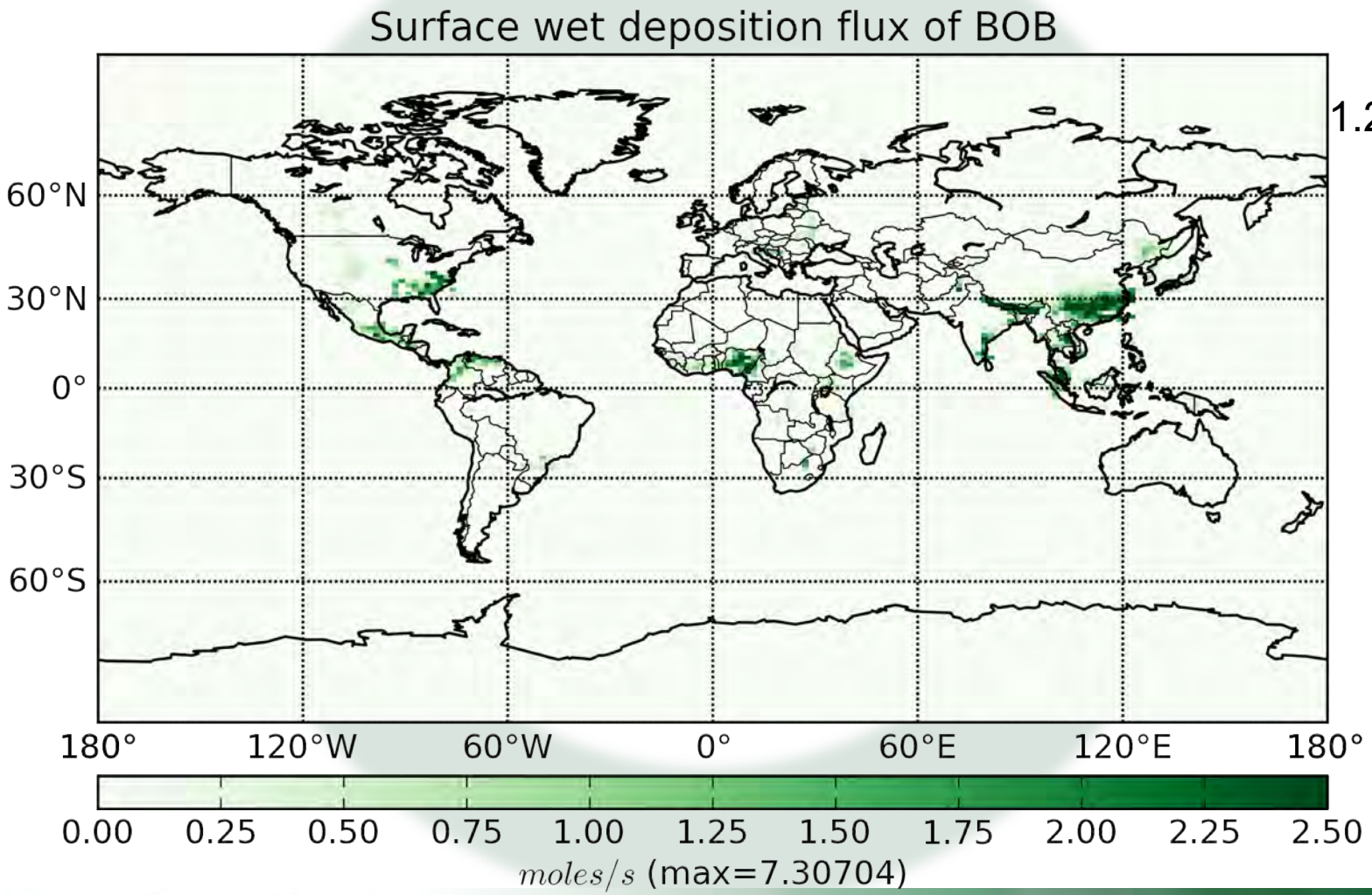
Tutorial 9: Adding new UKCA diagnostics



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

What should you now be able to do with UKCA?

After doing these 9 tutorials you should

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

Tutorial 10:
Examining Aerosol Impacts

Tutorial 10: Examining Aerosol Impacts

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 the change

ALICE + OH ➔ BOB

You should now work through the

10) Examining Aerosol Impacts

tutorial

Tutorial 10:
Examining Aerosol Impacts

Points to remember

1. STASH changes can be tricky, so take your time.
2. Python-Iris can be used to read and process UM data

Tutorial 11:
Developing a change for the trunk

Tutorial 11: Developing a change for the trunk

In this tutorial you are asked to

1. Test and fix a science change using rose-stem
2. Introduce a new control logical to the UKCA namelist
3. Make a test branch
4. Write documentation
5. Consider the steps of the review process

There are 3 UM releases a year, although code can be committed to the trunk at any time.

Points to remember

1. The UM development process seems quite complicated, but it exists to ensure that the code conforms to the standards required
2. There is a two-stage review process that check that the code does what it is supposed to do, and is written well
3. The code is only committed to the trunk by a member of the UM Systems Team once these reviews have been passed

Feedback

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

It would be very helpful for me if you could fill in the UKCA feedback form

More detailed comments can be emailed to me at

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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 ARCHER & NEXCS, and for those with a collaboration with the Met Office, on Monsoon2
- Recently, the Met Office have 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
  - UKCA will run “out of the box” in this environment from vn10.7

Virtual Machine

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]

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

Virtual Machine