

Using UKCA

Peter Braesicke

NCAS-Climate and

University of Cambridge

With thanks to: Luke Abraham, Jeff Cole, Rosalyn Hatcher, Lois Steenman-Clark and all UKCA users so far

Your contact: Luke.Abraham@atm.ch.cam.ac.uk

Preamble

- This talk is relevant for NCAS and NCAS affiliated UM/UKCA users.
- It is a general overview, not a comprehensive tutorial.
- Versions etc. have not been decided for the new shared HPC platform hosted at the Met Office under JCRP ...
- ... but NCAS and NCAS affiliated users will use the described procedure to create jobs and run the model on the shared HPC partition.
- Note: The shared HPC partition at the Met Office is relatively small and should be used to facilitate collaboration not to run “heavy” production (portability to NCAS HPC might be an issue ...)


UKCA HOME: a community resource!

UKCA Climate-Chemistry-Aerosol Community Model - Home - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.ukca.ac.uk/

Most Visited Getting Started Latest Headlines



UK Chemistry Aerosol Community Model

funded by the UK Meteorological Office and NERC Centres for Atmospheric Sciences
developed in collaboration with the UK Universities of Cambridge and Leeds

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UKCA Science


- Climate Chemistry Subproject
- Aerosol Subproject
- Air Quality Forecasting
- QUEST Theme1

Latest News


- Latest Results from the Model
- Progress Report

Welcome to UKCA


UKCA is a joint NCAS-Met Office programme funded by NCAS, GMR and DEFRA. Project partners are the Hadley Centre and the Universities of Cambridge and Leeds. Our objective is to develop, evaluate and make available a new UK community atmospheric chemistry-aerosol global model suitable for a range of topics in climate and environmental change research.




National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL



Met Office
Hadley Centre



UNIVERSITY OF LEEDS



UNIVERSITY OF CAMBRIDGE

Done

Today's talks will be here!


UKCA Mailing List

UKCA Climate-Chemistry-Aerosol Community Model - Mailing Lists - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.ukca.ac.uk/index.php?option=com_content&task=view&id=22&Itemid=35

Most Visited Getting Started Latest Headlines



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- Progress Report

Mailing Lists

UKCA Mailing Lists

There are two mailing lists associated with the UKCA project:

ukca-announce@atm.ch.cam.ac.uk ← this is intended for announcements related to UKCA such as new model releases, bugfixes, meetings and so on. It is expected to be a low volume list and all postings are moderated. It is hoped that all users will subscribe to this list. To subscribe, please fill in the simple form below.

Your email address:

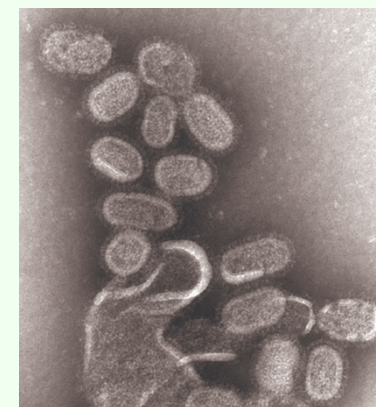
Subscribe ☒ Unsubscribe ☐

ukca-partners@atm.ch.cam.ac.uk: this is a private list for project partners only. Please contact Luke.Abraham@atm.ch.cam.ac.uk if you want to be added to this list.

[Back]

Release imminent...

... but slightly delayed by influenza:



Transmission electron microscopy picture of negatively stained influenza virions, magnified approximately 100,000 times.

Getting started

- PUMA account: to set-up the run
 - PUMA: **P**roviding **UM** **a**ccess
 - www.cms-ncas.ac.uk to apply for PUMA access
- Hector Account: to run the model
 - www.hector.ac.uk
 - NCAS accounts are managed by Lois Steenman-Clark, Reading
- Both services are accessible using ssh with X forwarding
 - `ssh -X -l username login.hector.ac.uk`
 - `ssh -X -l username puma.nerc.ac.uk`

NCAS-CMS and PUMA

National Centre for Atmospheric Science - Computational Modelling Services - Home - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://ncas-cms.nerc.ac.uk/

Most Visited Getting Started Latest Headlines

UM documentation

- ☐ UM Code
- ☐ PUMA Service
- ☐ Tools & Utilities
- ☐ Helpdesk
- ☐ Mesoscale Modelling
- ☐ Modelling Projects
- ☐ Related Links

HPC

- ☐ HPC Home
- ☐ HPC News
- ☐ HPC FAQs
- ☐ HPC Documentation
- ☐ HPC Accounting
- ☐ HPC Related Links

OTHER SERVICES

- ☐ Services Home
- ☐ Services FAQs
- ☐ Data
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- ☐ NCAS Publications
- ☐ NCAS Who's Who
- ☐ NCAS Climate News

ABOUT US

- ☐ Site Map

Welcome to NCAS Computational Modelling Services

The **National Centre for Atmospheric Science** (NCAS) provides a national capability in atmospheric science research through its research programmes and a facilities and support infrastructure.

The NCAS facilities and support infrastructure comprises of:

- High performance computing and modelling (CMS)
- Data archives (BADC)
- Airborne observations (FAAM)
- Ground based observations (UFAM)

Numerical Modelling

Development
Maintenance
Support
Training

Services

Information
Tools
Utilities

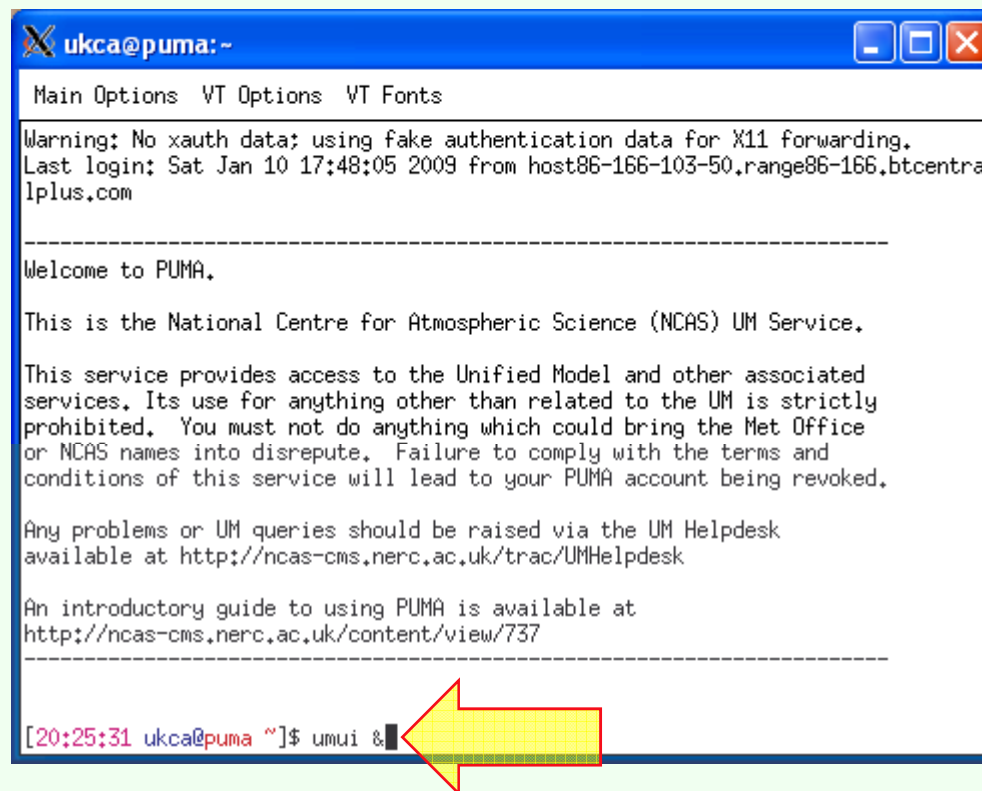
High Performance Computing

Allocation
Management
Help and advice

Last Updated (Monday, 07 January 2008)

On PUMA (provided by NCAS-CMS)

- Signing up to PUMA enables UM and UKCA access!



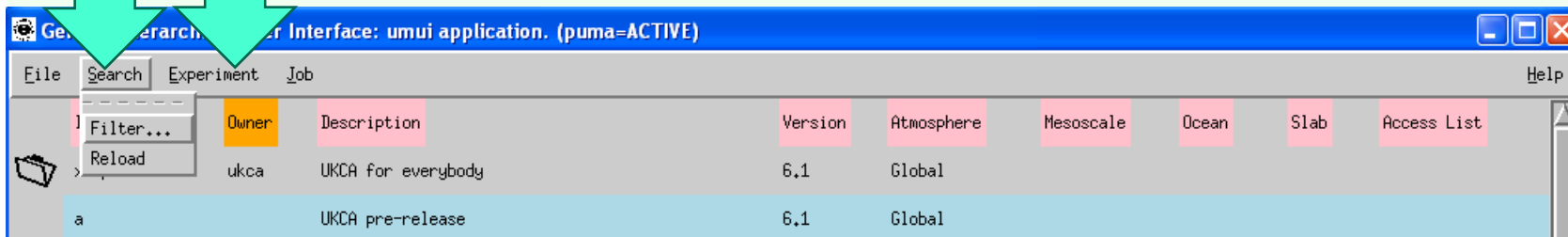
```
ukca@puma:~  
Main Options  VT Options  VT Fonts  
Warning: No xauth data; using fake authentication data for X11 forwarding.  
Last login: Sat Jan 10 17:48:05 2009 from host86-166-103-50.range86-166.btcentra  
lplus.com  
-----  
Welcome to PUMA.  
  
This is the National Centre for Atmospheric Science (NCAS) UM Service.  
  
This service provides access to the Unified Model and other associated  
services. Its use for anything other than related to the UM is strictly  
prohibited. You must not do anything which could bring the Met Office  
or NCAS names into disrepute. Failure to comply with the terms and  
conditions of this service will lead to your PUMA account being revoked.  
  
Any problems or UM queries should be raised via the UM Helpdesk  
available at http://ncas-cms.nerc.ac.uk/trac/UMHelpdesk  
  
An introductory guide to using PUMA is available at  
http://ncas-cms.nerc.ac.uk/content/view/737  
-----  
[20:25:31 ukca@puma ~]$ umui &
```

- Other services (e.g. ancillary file creation) require PUMA access! See e.g. **NCAS Ancillary File Service** on CMS web pages

UMUI + first steps

2

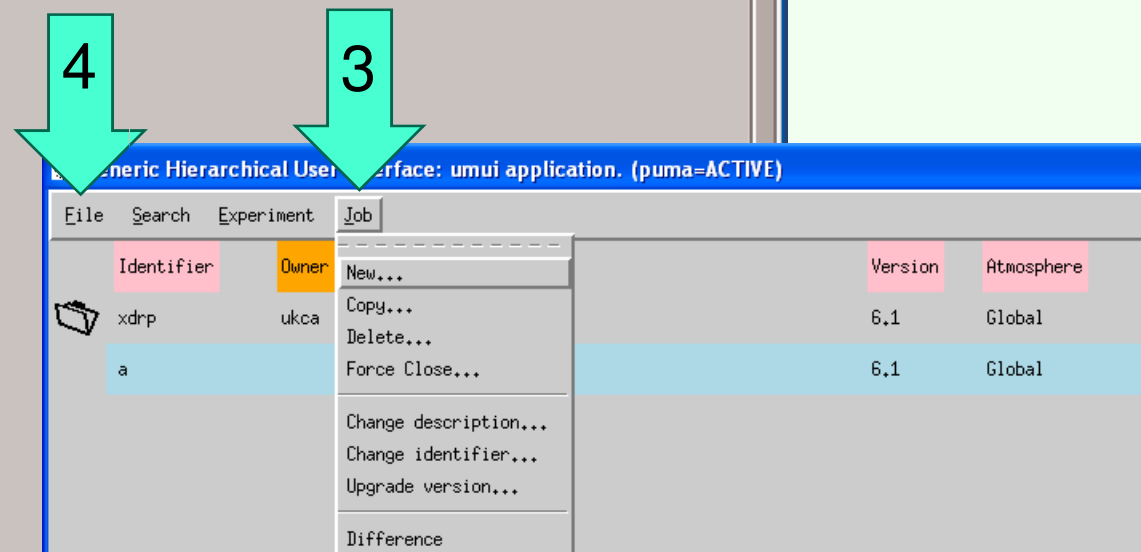
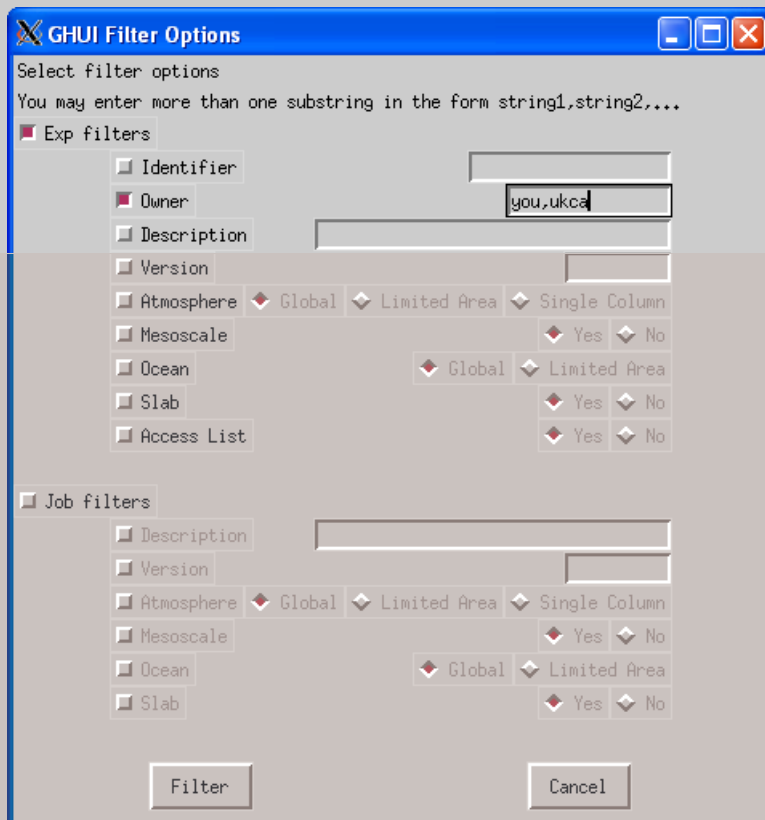
1



- 1) Create an experiment
- 2) Search for a template job
- 3) Copy the experiment
- 4) Edit the experiment

4

3



UKCA @ UM6.1

Generic Hierarchical User Interface: umui application. (puma=ACTIVE)

file
Search
Experiment
Job

Identifier	Owner	Description	Version	Atmosphere	Mes
xdrp	ukca	UKCA for everybody	6.1	Global	

umui application. Navigation of Job xdrp.a: "UKCA pre-release"

Model Selection

User Information and Target Machine

Sub-Model Independent

Sub-Model Configurations and Coupling

Reconfiguration

Atmosphere

Model Resolution and Domain

Model Configuration

Scientific Parameters and Sections

Section by section choices

Spec of trace gases

Data assimilation and temporal filtering

Ancillary and input data files

STASH

Control

Ocean GCM

Slab Ocean

Wave Model (Ocean surface waves)

Prognostic variable choices

Aerosols

Tracers

Run Mode

Atmospheric Tracers : Job xdrp.a: "UKCA pre-release"

☒ Do you want to include tracers in the atmosphere?

Mark the STASH tracer items to be included - these will have section 33 STASH numbers and STASHmaster entries.

The format of the left column is :-

<ITEM(TRACER NO; CONVENTIONAL USE)>

For the right column you should enter:-

0 - Do not include

1 - Include from dump

2 - Configure from ancillary tracer file (file needs attaching & see help)

3 - Update from aerosol climatology (file needs attaching)

Tracers

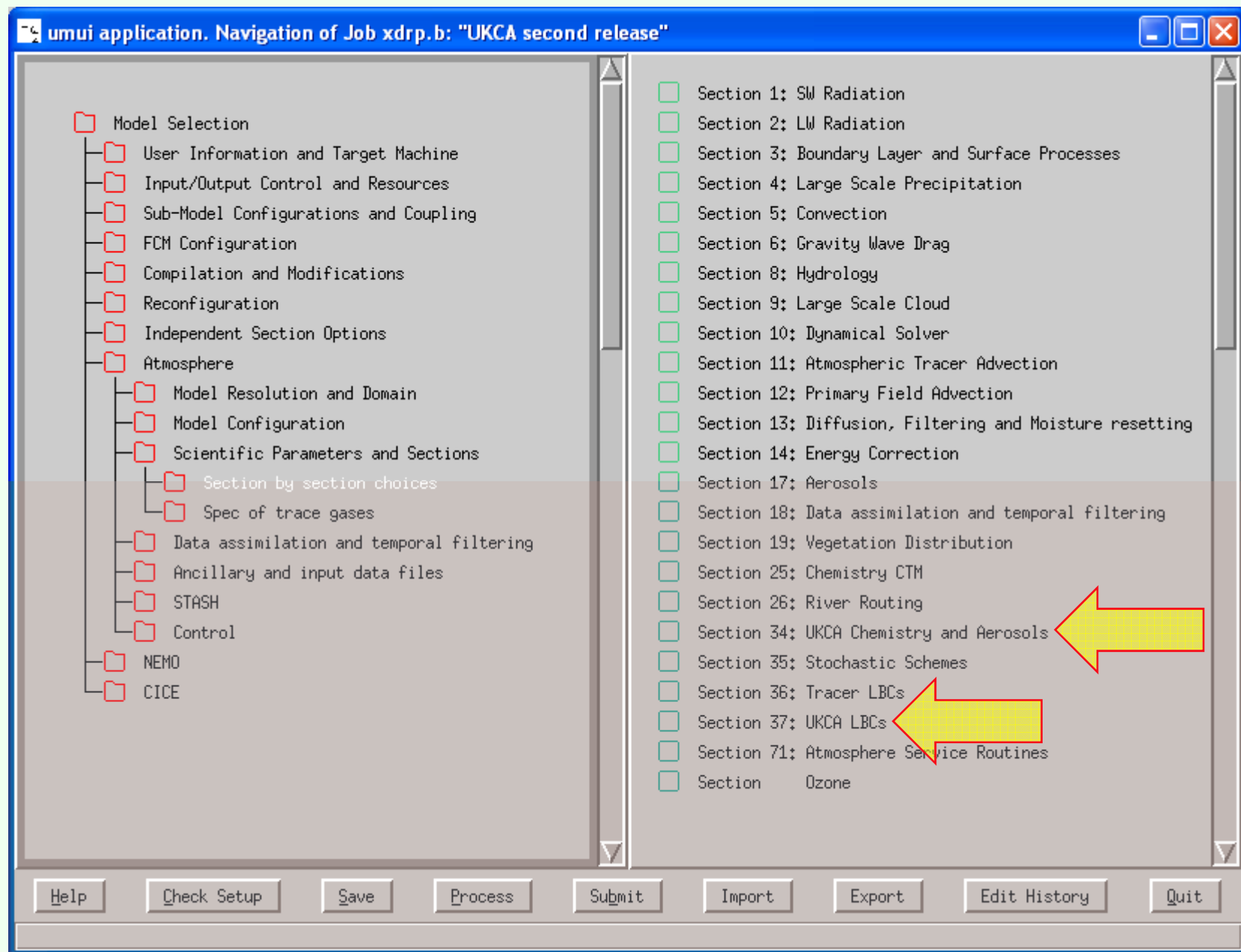
Tracers available	Select
1(01: TRACER_1)	1
2(02: TRACER_2)	1
3(03: TRACER_3)	1
4(04: TRACER_4)	1
5(05: TRACER_5)	1
6(06: TRACER_6)	1
7(07: TRACER_7)	1
8(08: TRACER_8)	1
9(09: TRACER_9)	1
10(10: TRACER_10)	1

Inert
Edit

☒ With boundary layer mixing of tracers

Number of atmospheric tracer levels
60

Chemistry is included. The number of tracer levels must equal the number of model levels



UKCA @ UM7.1

Generic Hierarchical User Interface: umui application. (puma=ACTIVE)

Identifier	Owner	Description	Version
xdrp	ukca	UKCA for everybody	7.1
a		UKCA first release	7.1
b		UKCA second release	7.1

Section 34: UKCA Chemistry and Aerosols : Job xdrp.b: "UKCA second release"

Choose the relevant section release

- <0A> UKCA not included.
- <1A> UKCA included.

Select Aerosol and Tracer Scheme(s)

- ☐ Use Family Chemical Tracers
- ☒ Use Separate Advected Tracer for Stratospheric H2O

umui application. Navigation of Job xdrp.b: "UKCA second release"

- Model Selection
 - User Information and Target Machine
 - Input/Output Control and Resources
 - Sub-Model Configurations and Coupling
 - FCM Configuration
 - Compilation and Modifications
 - Reconfiguration
 - Independent Section Options
 - Atmosphere
 - Model Resolution and Domain
 - Model Configuration
 - Scientific Parameters and Sections
 - Section by section choices
 - Spec of trace gases
 - Data assimilation and temporal filtering
 - Ancillary and input data files
 - STASH
 - Control
 - NEMO
 - CICE

- Prognostic variable choices
- Aerosols
- Atmospheric Tracers
- UKCA Chemistry and Aerosols
- Run Mode

- Not include
- Use 2D Photolysis Scheme
- Use FASTJ Photolysis Scheme
- No Chemical Scheme
- Standard Tropospheric Chemistry
- Isoprene + Tropospheric Chemistry
- Extended Tropospheric Chemistry
- Standard Stratospheric Chemistry

Atmospheric Tracers : Job xdrp.b: "UKCA second release"

☒ Do you want to include tracers in the atmosphere?

Mark the STASH tracer items to be included - these will have section 33 STASH numbers and STASHmaster entries.

The format of the left column is :-

<ITEM(TRACER NO; CONVENTIONAL USE)>

For the middle column you should enter:-

- 0 - Do not include
- 1 - Include from dump
- 2 - Configure from ancillary tracer file (file needs attaching & see help)
- 3 - Update from aerosol climatology (file needs attaching)

STASH: IO and coupling

STASH Panel ATMOS. Experiment xdrp, Job a @UM7.1

STASH Panel ATMOS. Experiment xdcy, Job b @UM6.1

STASH Panel ATMOS. Experiment xdcy, Job b

STASH Profiles Diagnostics Help

Time Profiles available

TDAYMN	TMIN	TMAX	TDAILY	TDMPMN	T24HDM	T90DAY	T6HMM	T6HDM	T12H	T30DAY	TTS
TALLTS	T5DYMN	TDAYMNGH	T3H	T3HMN	TDMPMN00	TDMPMN03	TDMPMN06	TDMPMN09	TDMPMN12	TDMPMN15	TDMPMN18
TDMPMN21	TMONMN	TACCEM	TACCCH	T10DAY	CCMGWD	TDAYMNRD	ANNMEAN	TMMDAILY			

Domain Profiles available

DIAG	DALLTH	DPBLTH	DP16	DSOIL	DBOTTH	D500	DPBLRH	DALLRH	DP50	DPHOT	SPECTROP
DBIMM96	DSPECIES	DGWDBOT	DALLCL	DTILE	D200	DPBLTH0	DALLTHXT	DA7ISCCP	DGWDTOP	DPSEUD	DBOT4
DP3	D100	CCMZMRH	CCMZM1L	CCMZM	CCMVALP	CCMVALZP	CCM3PLEV	CCM500HP	CCM2TH	CCMSURF	CCMLAND

Usage Profiles available

CCM10DAY	CCMDAILY	CCMMONTH	CCMMZM	UPCOUP	EPFLUX	TRACERS	UKCA_ANN	UKCADIA3	UKCADIA1	UPUKCA	UKCADIA2
----------	----------	----------	--------	--------	--------	---------	----------	----------	----------	--------	----------

STASH

Sec	Item	Diagnostic Name	Time	Domain	Usage	Include	Package	Available	User/System
4	223	SNOWFALL RATE OUT OF MODEL LEVELS	TALLTS	DALLCL	UPUKCA	Y	+	Y	SYSTEM
4	227	RAIN FRACTION OUT OF MODEL LEVELS	TALLTS	DALLCL	UPUKCA	Y	+	Y	SYSTEM
0	407	PRESSURE AT RHO LEVELS AFTER TS	TALLTS	DALLRH	UPUKCA	Y	+	Y	SYSTEM
0	406	EXNER PRESSURE AT THETA LEVELS	TALLTS	DALLTH	UPUKCA	Y	+	Y	SYSTEM
0	408	PRESSURE AT THETA LEVELS AFTER TS	TALLTS	DALLTH	UPUKCA	Y	+	Y	SYSTEM
0	409	SURFACE PRESSURE AFTER TIMESTEP	TALLTS	DIAG	UPUKCA	Y	+	Y	SYSTEM
1	201	NET DOWN SURFACE SW FLUX: SW TS ONLY	TALLTS	DIAG	UPUKCA	Y	+	Y	SYSTEM
1	235	TOTAL DOWNWARD SURFACE SW FLUX	TALLTS	DIAG	UPUKCA	Y	+	Y	SYSTEM
3	217	SURFACE HEAT FLUX W/M2	TALLTS	DIAG	UPUKCA	Y	+	Y	SYSTEM
30	453	Height at Tropopause Level	TALLTS	DIAG	UPUKCA	Y	+	Y	SYSTEM
Inert	Inert	Active	Active	Active	Active	Active	Active	Inert	Inert

Number of Diagnostics: 186

Over to HECTOR ...

1) Save the job
2) Check the job – only basic mistakes are picked up!
3) Process (creates namelists)
4) Submit to specified computer

Target Machine : Job xdrp.a: "UKCA pre-release"

◆ Compile, Link and Run on one platform
How is this Job to be run? ◆ Compile on one platform, Link and Run on another
◆ Compile and Link on one platform, Run on another

Note: At vn5.1, only 'Compile, Link and Run on one platform' should be used.
The other configurations have yet to be tested.

Compile, Link and Run the Job on the following machine:

◆ tx01 ◆ tx03 ◆ other

NEC node ◆ SX6 ◆ SX8

Other machine name ←

Target Machine user-id:
User-id

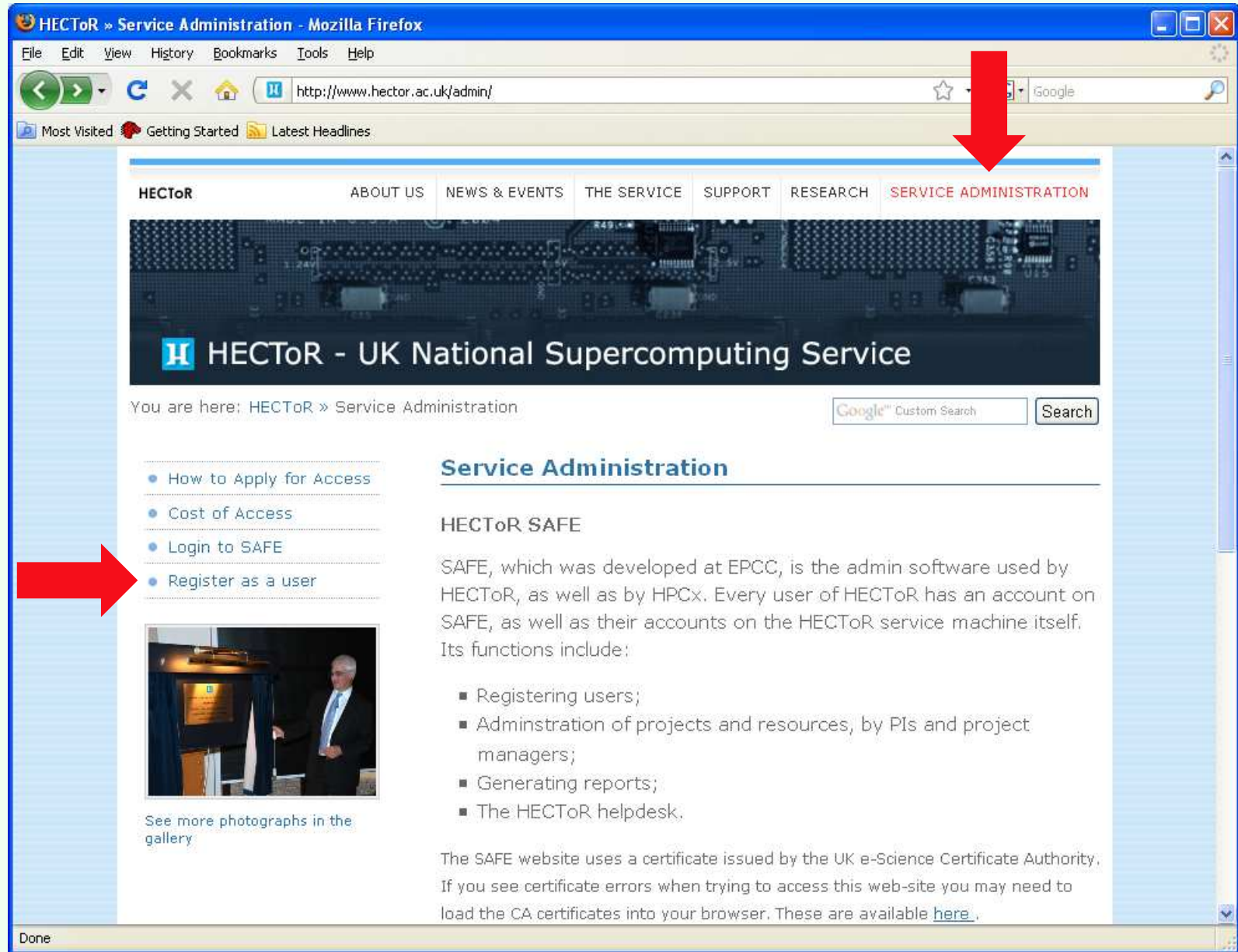
Running the job on the following machine type.

◆ Conventional Processor or using single node of a parallel machine
Machine type ◆ Shared-Memory Parallel (eg C90)
◆ Distributed-Memory Parallel (eg T3E or VPP)

Atmosphere or Wave submodel
Define the number of processors East-West. (Must be 1 or an even number).
Define the number of processors North-South

◆ F90 on Cray T3E / NEC SX-6
Supported Compiler ◆ F77 on Cray PVP
◆ Generic type

HECTOR



On HECTOR

```
peterb@nid15876:~
Main Options  VT Options  VT Fonts

not be used by users for the storing of any data

. Users should not leave backgrounded scripts running on login nodes. Any
processes running that are disconnected from a tty are liable for termination

. Please address all queries to "support@hector.ac.uk"

System is now running UNICOS/lc version 2.0.62

SERIAL BATCH JOBS NOW SUPPORTED - users should be using these for
large compilations, external file transfers, or any other activity
that currently makes significant use of "interactive" resources

07 01 09 Next maintenance session: 21 Jan/1200 - 21 Jan/2400
-----
PathScale PrgEnv loaded
peterb@nid15876:~> qstat -u peterb
sdb:

```

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	Elap S Time
192828.sdb	peterb	par:n32c	xdcyh051	456	1	1	--	12:00	R 09:23

```
peterb@nid15876:~>
```

Does it run?

Does it produce data?

```
peterb@nid15872:~
Main Options  VT Options  VT Fonts

. All users should note that the /work filesystem is unbacked-up scratch space
and should always be considered to be "at risk". Only /home filespace is
subject to a backup policy.

. It should be noted that /tmp filesystems are regularly purged and should
not be used by users for the storing of any data

. Users should not leave backgrounded scripts running on login nodes. Any
processes running that are disconnected from a tty are liable for termination

. Please address all queries to "support@hector.ac.uk"

System is now running UNICOS/lc version 2.0.62

SERIAL BATCH JOBS NOW SUPPORTED - users should be using these for
large compilations, external file transfers, or any other activity
that currently makes significant use of "interactive" resources

07 01 09 Next maintenance session: 21 Jan/1200 - 21 Jan/2400
-----
PathScale PrgEnv loaded
peterb@nid15872:~> xconv &
```

xconv on HECTOR (alternative convsh)

Xconv Version 1.91 (16-February-2006)

Output file name: Output format:

	nx	ny	nz	nt	Field title	longitude (degrees_east)
0	: 96	73	120	4	U COMPNT OF WIND AFTER TIMESTEP	1.875000
1	: 96	72	120	4	V COMPNT OF WIND AFTER TIMESTEP	5.625000
2	: 96	73	480	4	THETA AFTER TIMESTEP	9.375000
3	: 96	73	4	4	SOIL MOISTURE CONTENT IN A LAYER	13.125000
4	: 96	73	480	4	SPECIFIC HUMIDITY AFTER TIMESTEP	16.875000
5	: 96	73	480	4	QCF AFTER TIMESTEP	20.625000
6	: 96	73	1	4	CONV CLOUD BASE LEVEL NO. AFTER TS	24.375000
7	: 96	73	1	4	CONV CLOUD TOP LEVEL NO. AFTER TS	28.125000
8	: 96	73	1	4	CONV CLOUD LIQUID WATER PATH	31.875000
9	: 96	73	1	4	SILHOUETTE OROGRAPHIC ROUGHNESS	35.625000
10	: 96	73	1	4	HALF OF (PEAK TO TROUGH HT OF OROG)	39.375000
11	: 96	73	4	4	DEEP SOIL TEMP AFTER TIMESTEP	43.125000
12	: 96	73	1	4	CANOPY WATER AFTER TIMESTEP KG/M2	46.875000
13	: 96	73	1	4	SNOW AMOUNT OVER LAND AFT TSTP KG/M2	50.625000
14	: 96	73	1	4	SURFACE TEMPERATURE AFTER TIMESTEP	54.375000
15	: 96	73	1	4	BOUNDARY LAYER DEPTH AFTER TIMESTEP	58.125000
16	: 96	73	1	4	ROUGHNESS LENGTH AFTER TIMESTEP	61.875000
17	: 96	73	1	4	SURFACE ZONAL CURRENT AFTER TIMESTEP	65.625000
18	: 96	72	1	4	SURFACE MERID CURRENT AFTER TIMESTEP	69.375000
19	: 96	73	1	4	LAND MASK (No halo) (LAND=TRUE)	73.125000
20	: 96	73	1	4	FRAC OF SEA ICE IN SEA AFTER TSTEP	76.875000
21	: 96	73	1	4	SEA ICE DEPTH (MEAN OVER ICE) M	80.625000
22	: 96	73	1	4	OROGRAPHY (/STRAT LOWER BC)	84.375000
23	: 96	73	1	4	STANDARD DEVIATION OF OROGRAPHY	88.125000

Output messages Field information

Data and tools

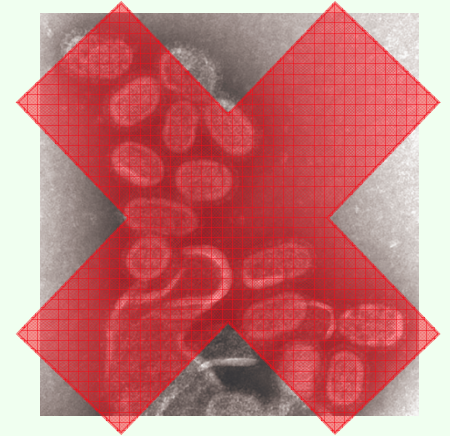
- Data required to run the model (on ukca work):
 - Initial conditions: dumps and ancillary files
 - Boundary conditions: ancillary files, e.g. SSTs, sea-ice, emissions, and many more
 - Files to constrain the nudged model: netcdf format, pre-processed ECMWF and Met Office
- Tools (on ukca home or um home)
 - Data processing
 - Simple plotting
 - User contributions (Please contribute!)

Note

- Much detail has been omitted ...
- ... but will be mentioned in the forthcoming documentation.
- This talk did not cover specific background requirements for changing the chemistry or the aerosol scheme!
- Default jobs will be provided via the ukca account on PUMA and should be run unchanged first! Obviously only for a short integration period ... (include “ukca” in your umui filter settings)
- After the default job run, start with your modifications ...
- ... and enjoy the new science!

What next?

- 1) Register with mailing list:
`ukca-announce@atm.ch.cam.ac.uk`
- 2) Announcement of availability soon ...
- 3) Point of contact: Luke Abraham
`Luke.Abraham@atm.ch.cam.ac.uk`
- 4) Read documentation on www.cms-ncas.ac.uk and
www.ukca.ac.uk
- 5) Try it, enjoy it, ...
- 6) ... and provide feedback, please!





www.ukca.ac.uk

Thank you
for your
attention!



UKCA Launch, 12 January 2008

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