

# NCAS-CMS

Computer Modelling Services

A whistle-stop tour of activities

- Personnel
- Core activities
- HECToR
- ARCHER
- Projects

Simon Wilson



Model Support and Performance Specialist

Simon Read



UKESM1 core team – diagnostics

Karthee Sivalingam



JWCRP Porting, new architectures, high-res support

Jeff Cole



Model Support and Software Tools Specialist

Andy Heaps



System Administration and Visualisation Specialist

## Computational Modelling Services

A Service for all UK Academic users

Bryan Lawrence



Director of Models and Data

Charles Roberts



CF-Python/PAGODA

Rosalyn Hatcher



Software Management Specialist  
MMG

William McGinty



Modelling Support for the mesoscale community  
Data

David Hassell



Software Tools specialist – CF-Python - IS-ENES2

Grenville Lister



CMS local manager and modelling and HPC Support

Luke Abraham



UKCA development and support

Annette Osprey



Modelling Support for Earth System Models, NEMO  
HPC futures

# NCAS Computational Modelling Service (CMS) Group

*providing services to the UK academic modelling community*

What services does NCAS-CMS provide?

## Access to models and software

- **Met Office Models – porting, installation and support**
  - Unified Model (UM) (vns [4.5], 6.1, 7.3, ...8.6...)
  - NEMO, CICE, OASIS, JULES
  - UKCA, LEM, SCM
- **PUMA**
  - Academic central facility for UM code, experiments, HPC access
- **Software tools for data manipulation and analysis**
  - xconv, xancil, JVIEW, NDDIAG
  - Metadata and visualization
  - Central Ancillary Program (CAP)
  - CF-Python, CF-Plot

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- **JASMIN**

- Super-data-cluster at BADC
- Distributed component – data storage

## *Access to High Performance Computing (HPC) facilities*

- **ARCHER – the national HPC service**

- Cray XC30 + Research Data Facility (RDF)
- Service provision

UM + UMUI vns 6.1 6.6.3 7.3  
7.8 8.2 8.4 8.5 8.6

- **MONSooN**

- IBM joint NERC/UKMO supercomputer

UM + UMUI 6.6.3 ...8.4 8.5 8.6

- **Polaris**

- N8 consortium machine at Leeds

4.5, 6.6.3, 7.3, 8.4

- **HPC Wales**

- <http://www.met.reading.ac.uk/~ros/sphinx/software/build/hpcwales.html>

8.5

- **NOC cluster (coupled configuration)**

- **Tests on innovative HPC worldwide**

- CURIE Bull (France)
- GPU's

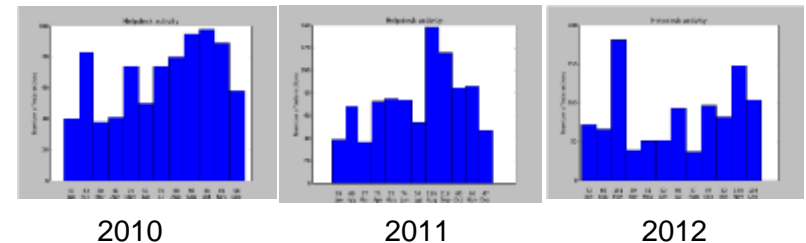
# NCAS Computational Modelling Service (CMS) Group

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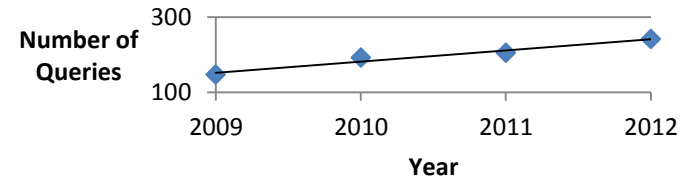
What services does NCAS-CMS provide?

## Modelling support and access to information

- **Helpdesk**
  - UM, HPC, software, infrastructure
  - searchable
- **CMS website**
  - Documentation, FAQ's, key updates



CMS Helpdesk queries



## Training and documentation

- **UM training (NERC funded)**
  - Basic introduction + hands-on on ARCHER
- **IDL/FCM/CF-Python/CF-Plot user guides**

“I think the course was flawless”  
“All of them were magnificent”  
Feedback from the York UM Training March 2014

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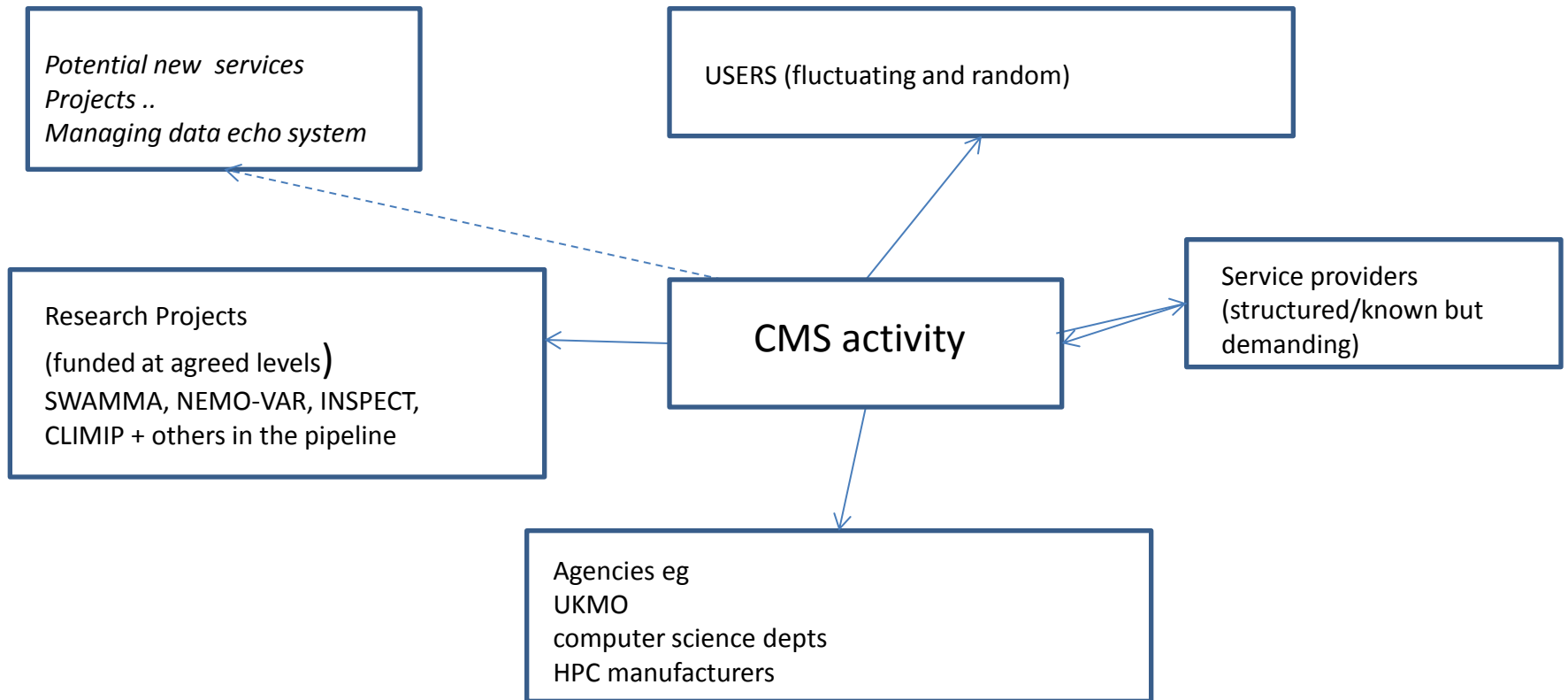
## Collaboration and interaction

- **ac.uk**
- **UKMO**
  - Users
  - MONSooN/UM installations
  - Rose
  - Technical Infrastructure
- **EPCC**
  - ARCHER
  - RDF
- **NERC**
  - HPC management
- **BADC**
  - Data/JASMIN
- **ECMWF**
  - OpenIFS
- **ARC (Australia)**
  - CMS

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## Tensioning CMS



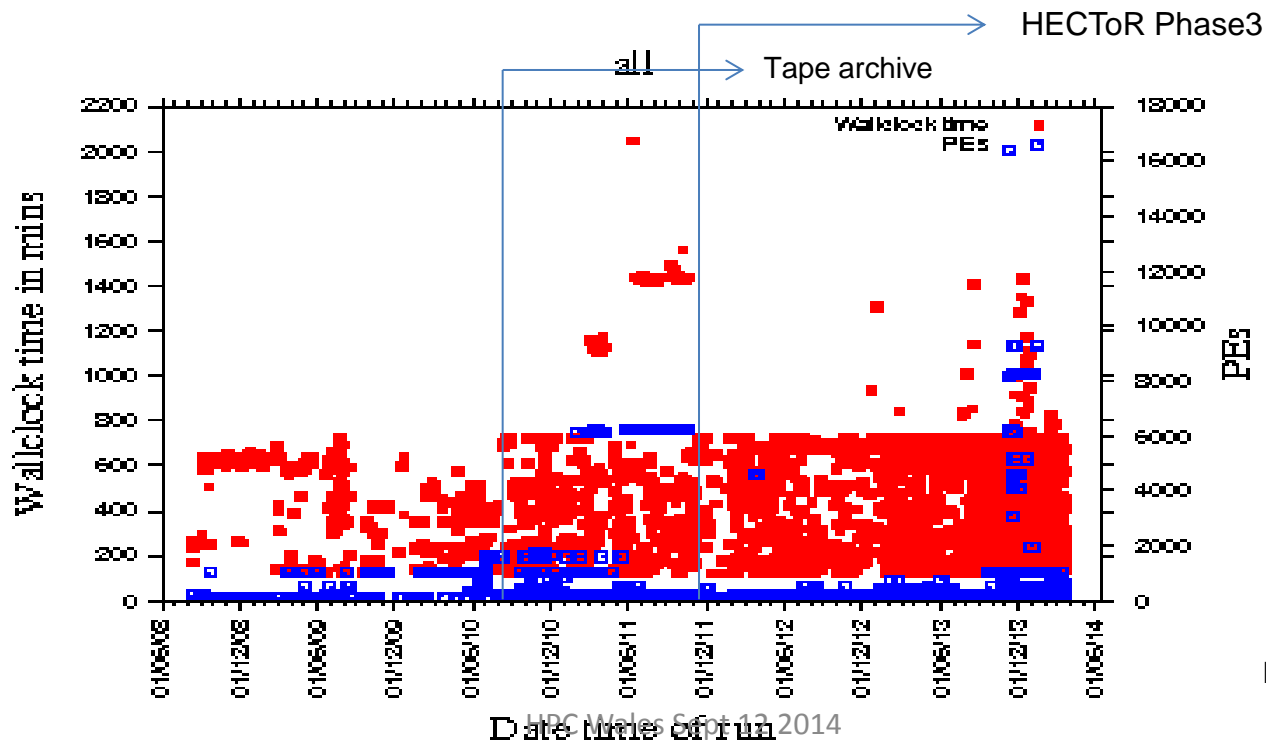


- Personnel
- Core activities
- **HECToR**
- ARCHER
  - RDF
- Projects

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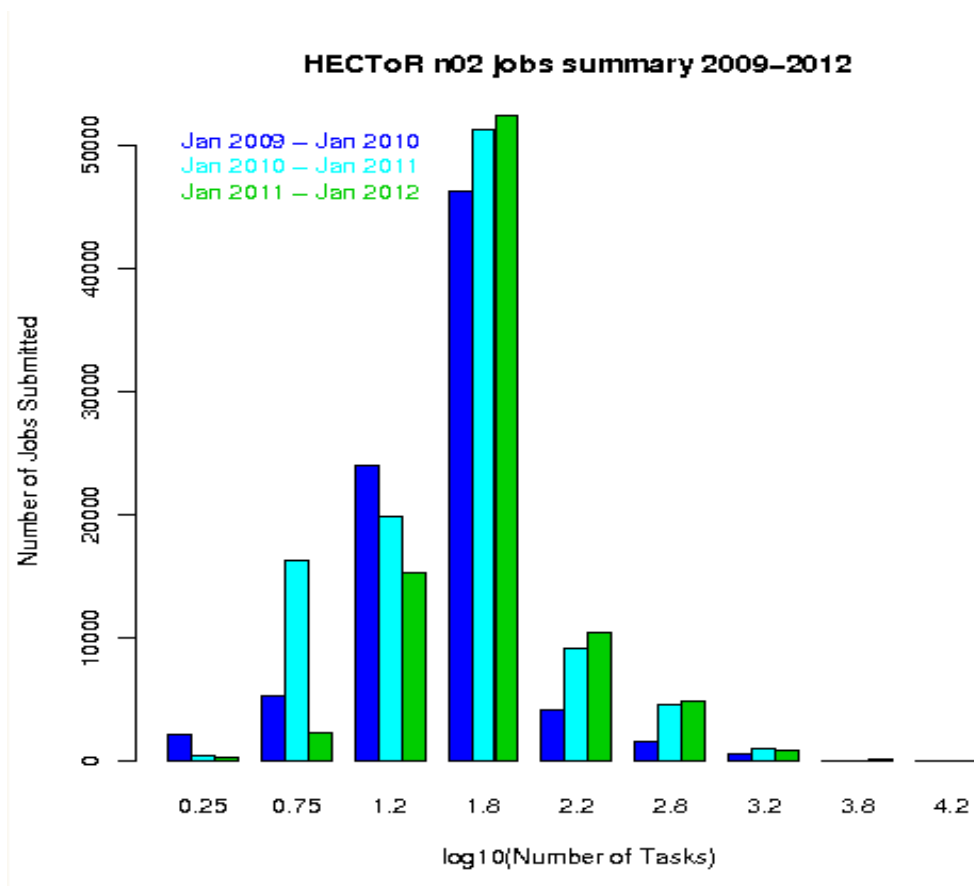
- Hector switched off March 24<sup>th</sup>
- Data transfer appears to have been relatively uneventful (RDF)
  - ~300Tb /work (by users)
  - ~450Tb tape archive (by HECToR)
- Heavy usage in the final few weeks of its life



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## Usage over time n02



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## **ARCHER (Advanced Research Computing High End Resource)**

- Funded by UK Research Councils
- Operated by HPCX, EPCC
- EPSRC managing agent
- NERC 22% share

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## ARCHER (Advanced Research Computing High End Resource)

- Live Dec 2014
- 2632 standard memory nodes (63,168 cores)
- 376 high memory nodes (9,024 cores)
- total of 3008 compute nodes (72,192 cores)
- 32 Service nodes/8 login nodes
- 2 PP machines (40 processors each)
- Aries interconnect
- n02 share - 1.4 PB parallel disc (Lustre) available to compute nodes (not backed up)
- Research Data Facility (RDF) – 13.8PB (increasing to 23PB)
- Phase 2 about to arrive



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## ARCHER (Advanced Research Computing High End Resource)



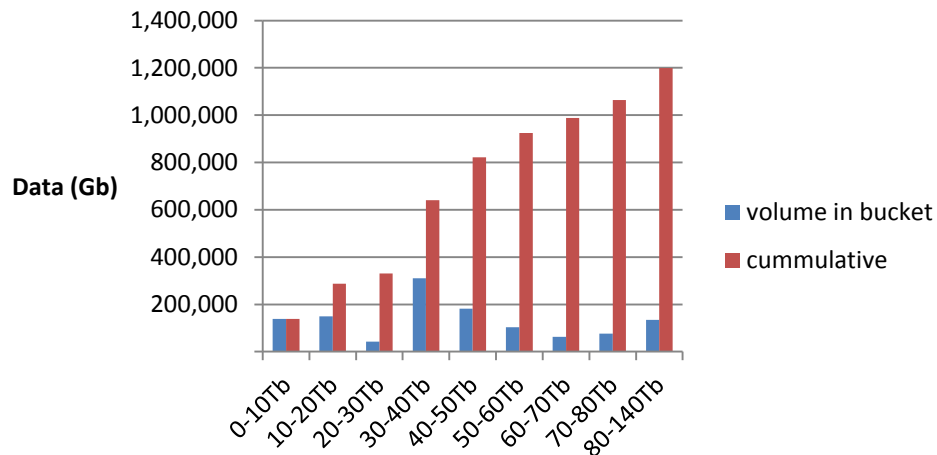
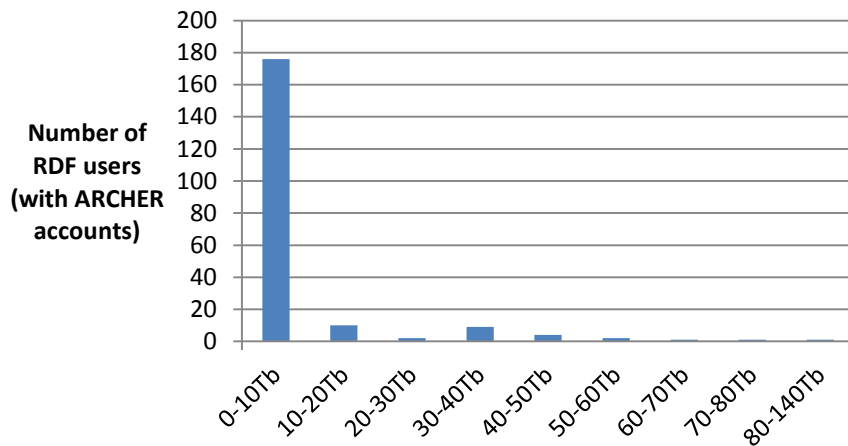
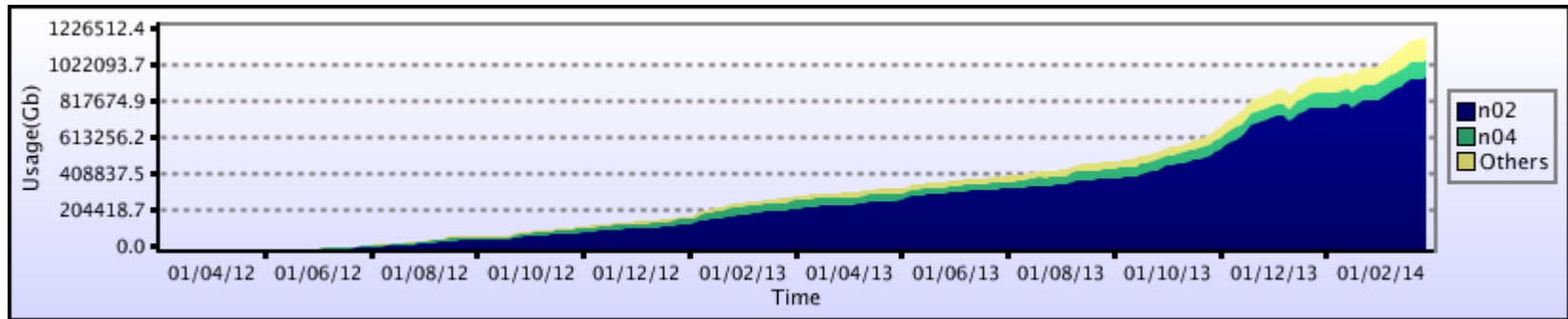
### HECToR-ARCHER Comparison

UM Version	ARCHER compiler	Description	EWxNS	Run Length	Dump Frequency	HECToR Job Id	HECToR Walltime	ARCHER Job Id	ARCHER Walltime
6.1	cce	HIGEM1a	8x15	10 days	10 days	xjazn	01:13:46	xjazo	00:30:22
6.1	intel	HIGEM1a	8x15	10 days	10 days	xjazn	01:13:46	xjazp	00:29:33
6.6.3	cce	HadGEM2-AMIP	12x8	10 days	1 day	xjgcd	00:18:27	xjgcc	00:07:21
6.6.3	intel	HadGEM2-AMIP	12x8	10 days	1 day	xjgcg	00:18:27	xjgce	00:07:52
6.6.3	cce	HadGEM2-CC60	12x8	30 days	10 day	xjgcg	01:43:00	xjgcf	00:44:31
6.6.3	cce	HadGEM2-AO	12x8	30 days	10 day	xjgcy	00:53:57	xjgch	00:23:58
6.6.3	cce	HadGEM2-AO	6x8	30 days	10 day			xjgch	00:41:14
6.6.3	cce	HadGEM2-AO	6x4	30 days	10 day			xjgch	01:16:00
6.6.3	cce	HadGEM2-ES	12x8	3 days	1 day	xjgct	00:12:58	xjgcu	00:05:32
7.3	cce	HadGEM3-A r2.0	4x6	10 days	10 days	xehif	01:50:42	xjeya	00:54:40
7.3	cce	⇒ UKCA TropIsop N48L60	8x9	10 days	10 days	xjfly (c.f. xfvf)	00:21:52	xjflj (c.f. xfvfd)	00:09:11
8.2	cce	GA4.0 N96 AMIP OpenMP(2 Thds)	8x12	10 days	10 days	xgwtg	00:23:48	xjeye	00:11:56
8.2	cce	GO5.0 ORCA025 (NEMO vn3.4)	8x12	5 days	5 days	xiyla	01:16:56	xiylc	00:23:03
8.2	cce	PS30 Global	6x16(x4)	1 days	6 hrs	xiekb	03:26:20	xjkgb	01:29:09
8.4	cce	N96 UKCA OpenMP	24x16	10 days	10 day			xjnjc	00:15:52
8.4	cce	HG3A GA4.0 OpenMP (2 Thds)	8x12	10 days	10 days	xgwtq	00:21:10	xjeyf	00:10:03
8.5	cce	N512 GA6.0 OpenMP (2 Thds)	32x32	1 day	10 days	xjang	00:20:10	xjano	00:10:38
8.5	cce	idealized 1km L60	36x36	1 hr	1 hr	xjaru	00:19:21	xjarf	00:08:23
8.5	cce	idealized 1km L60	36x12	1 hr	1 hr			xjarf	00:17:47
8.5	cce	idealized 1km L60	16x24	1 hr	1 hr			xjarf	00:19:00
8.5	cce	idealized 1km L60	16x12	1 hr	1 hr			xjarf	00:34:14
8.5	intel	idealized 1km L60	26x26	1 hr	1 hr	xjagu	00:10:21	xjard	00:10:57

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**RDF (Research Data Facility) 13.8PB NERC share 22% (3PB)**



Group quota management soon – joined up with JASMIN

RDF compute cluster soon-ish

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## Compute/Data management

- Local
  - 200 cores
  - 1PB disc
  - Servers - arcacia, plane, robinia, gingko, mikan, oak, poplar, quince, marula, hawthorn, sunspot, pinggwo, greenwood, pine, iguazu, niagara, mango, hickory, chestnut, jasmin1-jasmin6, um1, um2, puma, bill, birch, laburnum, hazel, fir, willow
- ARCHER
  - 220 users
  - 2.1PB (RDF) + 300TB (work)
- PUMA
  - 600 users



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## HPC management

NERC { n01 – Ocean/Shelf Seas  
n02 – Atmospheric and Polar  
n03 – Solid Earth

- Share 2.1 BAU/yr
- NCAS (NC) core - 10 subcategories - 700 MAU
- NERC grants/fellowships – 35 individual projects – 200 MAU

- Personnel
- Core activities
- HECToR
- ARCHER
- **Projects**

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## Projects

### UM-netCDF

- Jeff Cole - UM to write CF-NetCDF directly (eliminate the need for a great deal of effort converting data formats)

### CLIMIP

- Simon (W) is working on Climate Model Initialization and Improvement using Particle Filters

### Rose

- Ros and Annette are working to implement the new UM infrastructure on ARCHER/MONSooN and other architectures

### Modelling model performance

- Annette is developing a model to predict wall-clock times for applications running on high-performance computers

### CF Python

- David is developing the Python implementation of the CF data model + tools – Charles starting here

### CF Plot

- Andy's CF-Plot

### CAP

- Reengineering the CAP interface upgrading maintenance procedures – shared repository test

### OpenIFS

- CMS will host OpenIFS for the ac.uk community – 6 month dCSE project award to implement parallel I/O

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UM performance improvements

Cray Reveal – adding OpenMP sections



UM Version	Job desc	UMUI	Installed	NRUN	CRUN
8.5	N512 L180 GA 6.0	xjanp	Yes	Passed	Passed
8.5	N216 L180 GA 6.0	xjlef	Yes	Passed	Passed
8.4	N512 L85 GA 6.0	xjanu	Yes	Passed	Passed
8.6	GA4.0 & UKCA CheST & GLOMAP	xjnjb	Yes	Passed - Only for the same PE decomposition	Failed (expect it to Not bit-compare- Mohit Dalvi)
8.5	GC2 N96/Ora1	xjnja	Yes	Passed	Passed
8.5	GA6.0 N216 antib	xjlee	Yes	Passed	Passed
8.5	GA6.0 N95 antia	xjlen	No	-	-

Job porting (UKESM1) – Karthee & Matthew Hambley (MO)  
Running the High-res GW experiments (BNL....)

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## CF-Python (David, Charles)

Implements the CF data model for the reading, writing and processing of data and its metadata.

- Read CF-netCDF, CFA-netCDF and PP format files.
- Create CF fields.
- Aggregate collections of fields
- Write fields to CF-netCDF and CFA-netCDF files on disk.
- Create, delete and modify a field's data and metadata.
- Select fields according to their metadata.
- Subspace a field's data to create a new field.
- Perform broadcastable, metadata-aware arithmetic
- Collapse fields by statistical operations.
- Sensibly deal with date-time data.

### Reading files

The `cf.read` function will read CF-netCDF and CFA-netCDF files (or URLs if DAP access is enabled) and Met Office (UK) PP format files from disk and return their contents as a field list, i.e. an ordered collection of fields stored in a `cf.FieldList` object:

```
%% f = cf.read('data.nc')
%% type(f)
<class 'cf.FieldList'>
%% f
<CF Field: air_pressure(grid_latitude(30), grid_longitude(24)) Pa>
<CF Field: u_wind(height(10), grid_latitude(26), grid_longitude(24)) m s-1>
<CF Field: v_wind(height(10), grid_latitude(26), grid_longitude(24)) m s-1>
<CF Field: air_potential_temperature(height(10), grid_latitude(26), grid_longitude(24)) K>
%% f[1]
<CF Field: air_potential_temperature(height(10), grid_latitude(26), grid_longitude(24)) K>
```

The `cf.read` function always returns a field list as opposed to a field. If a single field as a `cf.Field` object is required, then the `cf.read` function (or rather its returned field list) may be indexed:

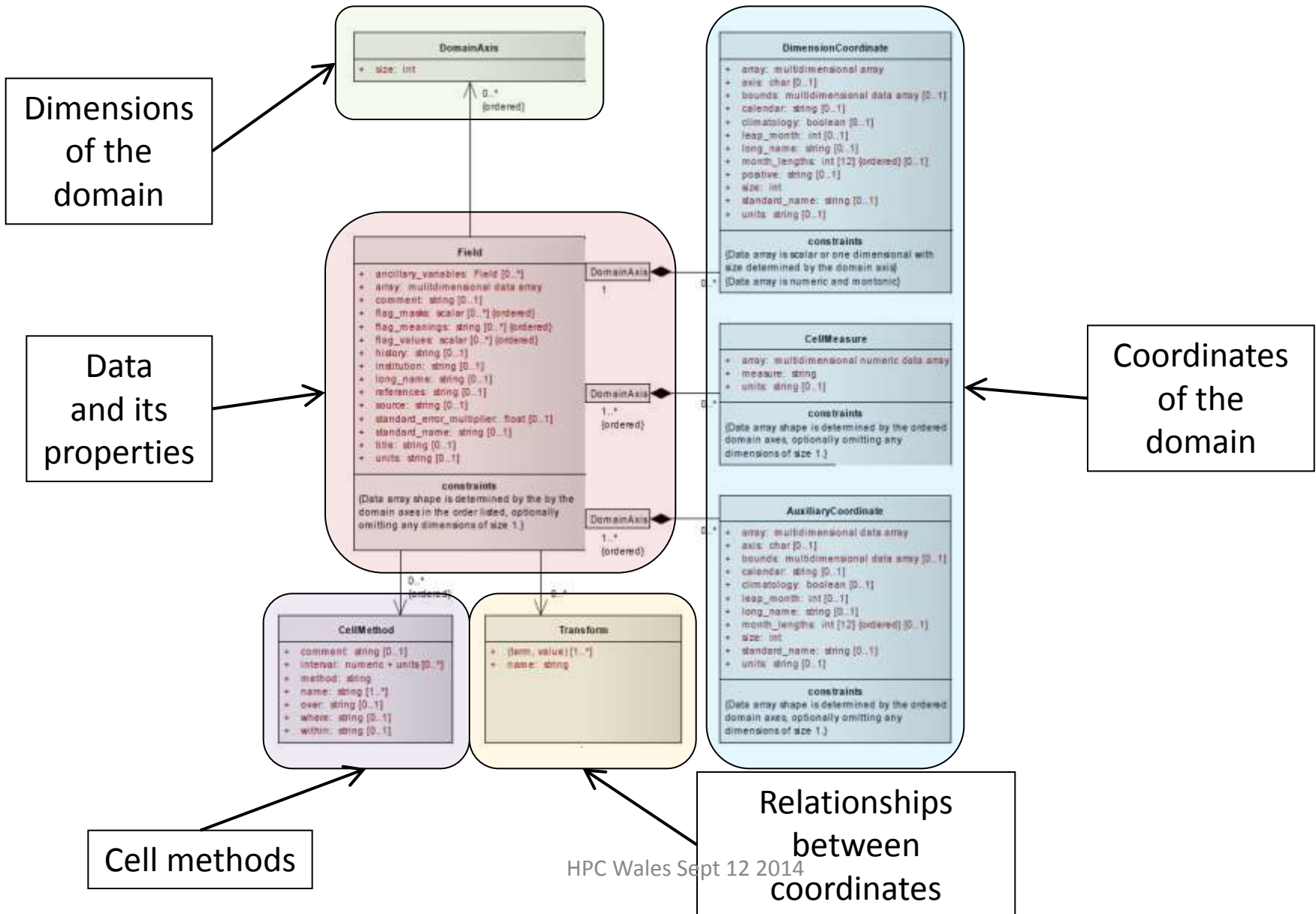
```
%% f = cf.read('data.nc')[0]
```

Multiple files may be read at once by using Unix shell wildcard characters in file names or providing a sequence of files:

```
%% f = cf.read(['*.nc'])
%% f = cf.read(['file1.nc', 'file2.nc'])
%% f = cf.read(['dir/*.*'])
%% f = cf.read(['file1.nc', 'file2.nc', 'file3.nc'])
```

All of the above use Large Amounts of Massive Arrays (LAMA) functionality

# Diagram of the CF data model

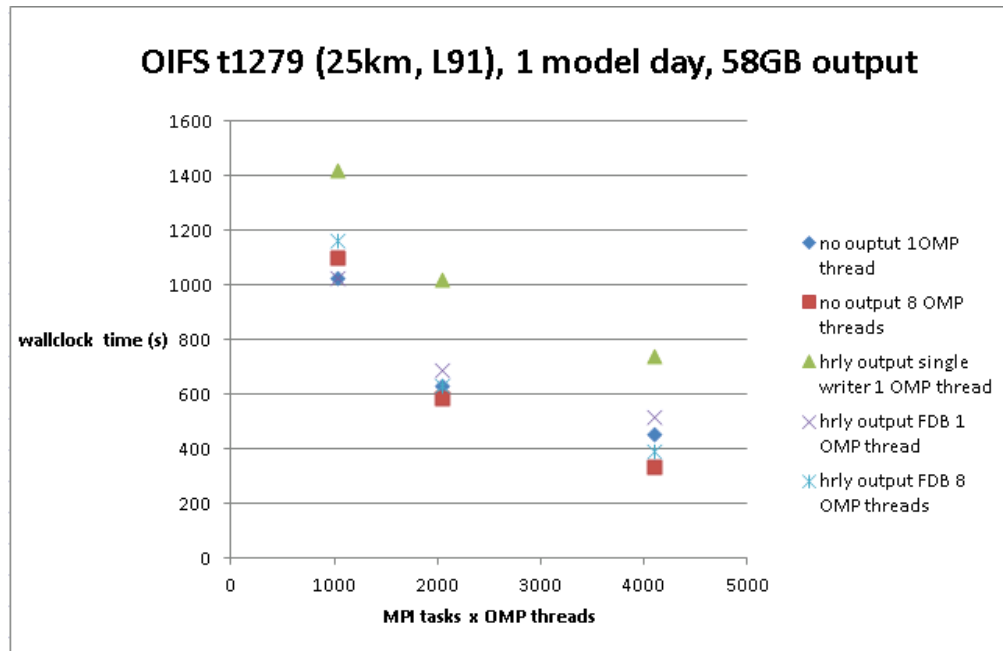


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## OpenIFS

- CMS 6 month dCSE project award to implement parallel I/O
  - Mark Richardson (NAG) , Glenn Carver (ECMWF), Rosalyn Hatcher, Grenville Lister



OpenIFS + FDB on HECToR

PUMA OpenIFS repository