Climate Science and NCAS CMS: An intro!

Scientific context and some examples of the activities of one of the oldest University based RSE groups in the UK.

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NCAS and the University of Reading





Outline

- Climate Modelling: the inexorable consumer of computing and producer of data.
 - The role of resolution, complexity and ensembles.
- What supporting (academic) climate modelling in the UK requires
 - An intro to CMS itself and the helpdesk
- Some example activities:
 - Modelling at Scale: CANARI
 - Modelling Futures: Preparing for Grace-Hopper
 - Models and Data: Intercomparison with TWINE-VISION
 - Data: A pure python HDF reader, pyfive





Given knowledge of state at every grid point at time t, calculate at every grid point state at $t + \Delta t$.

Many points, much state, integrated for years with timestep of *o(minutes)*!



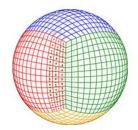
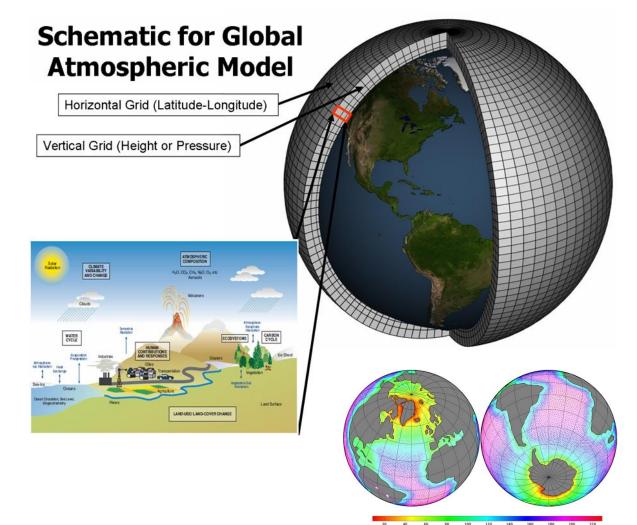


Image credits for tho sel know. http://dx.doi.org/10.48550/arXiv.2508.17462 https://www.gfdl.noaa.gov/fv3-grids/ https://doi.org/10.1016/j.dynatmoce.2017.05.003



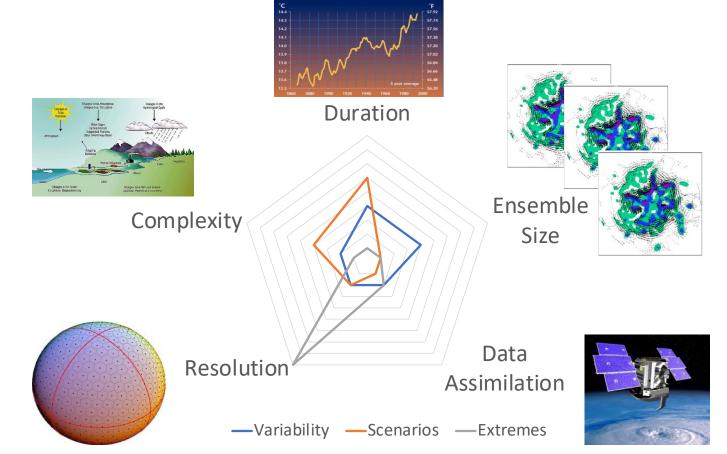


Give me more compute?

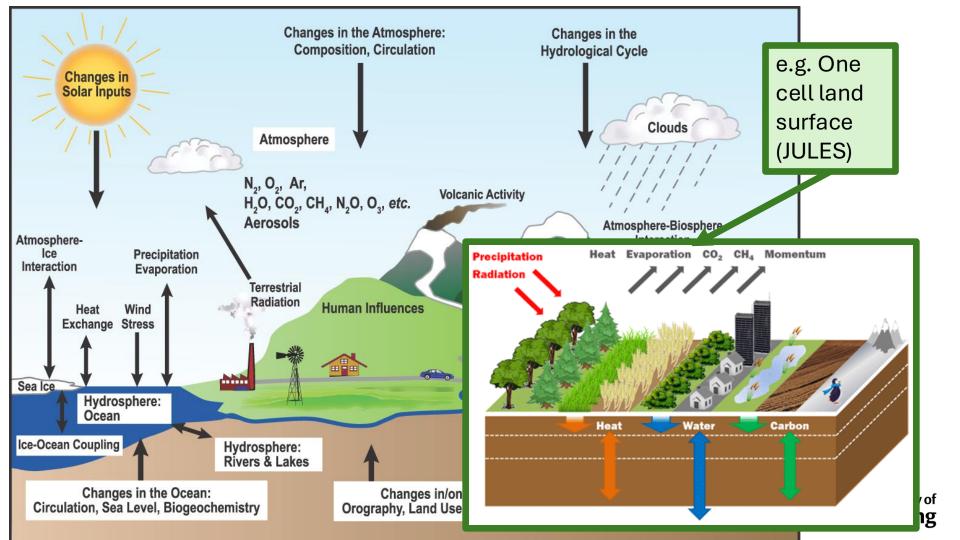
WE can't have it all!

WE need to spend compute on the key aspects of the problem.

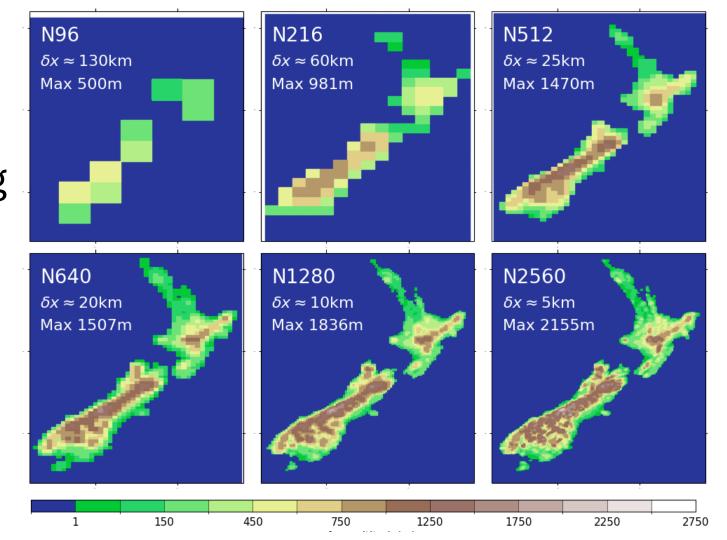
Which are?







Attempting a visceral feeling for resolution



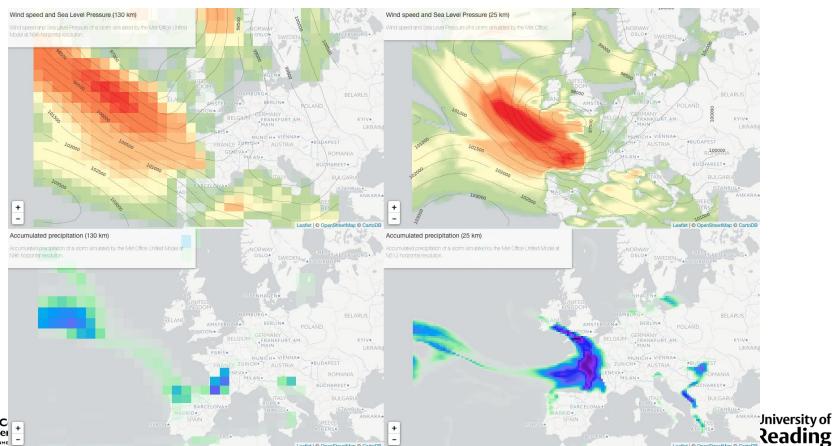








P-L. Vidale (PI NCAS HCRCM)



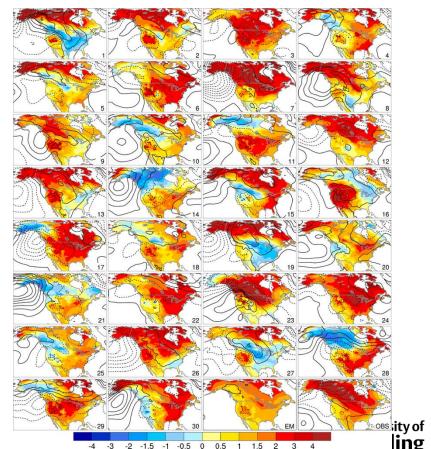


What is a large ensemble?

- A single climate model simulation exhibits variability due to natural internal atmosphere/ocean processes (e.g. ENSO)
- Variability becomes even more important on regional scales:
 - 50-year temperature trends over North America 1963–2012 in 30 historical simulations
 - Warming due to greenhouse gases is clear, but internal variability is also large



From Deser et al., 2016, JClim



What is a large ensemble?

From Deser et al., 2016, JClim

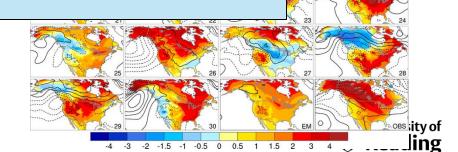
 A single climate model simulation exhibits variability due to natural

internal a (e.g. ENS

A large ensemble is a collection of climate model simulations which all

- Variability important
 - 50-yea
 North
 histori
- Follow the same experiment (protocol)
- Aim to sample internal variability independently and exhaustively
- Warming une to greenhouse gases is clear, but internal variability is also large



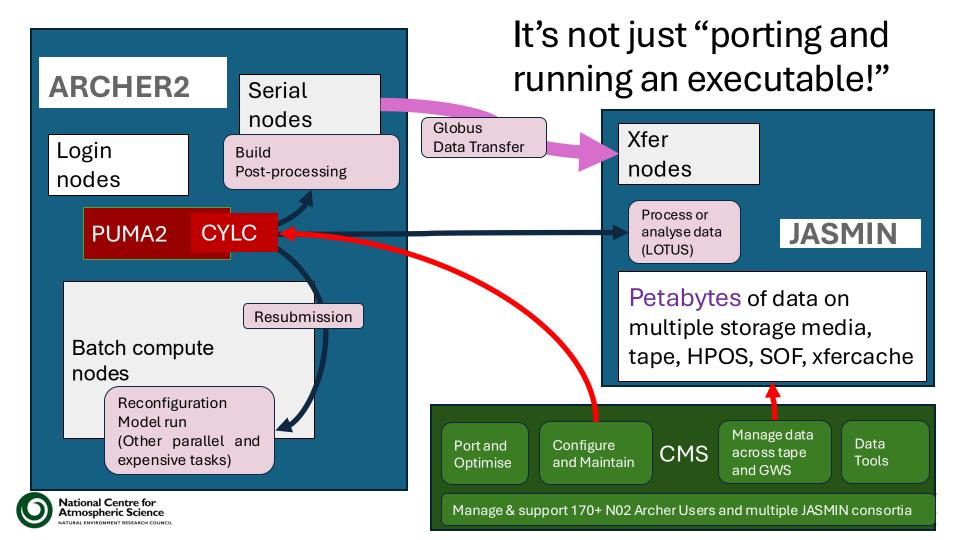


Coupled Ocean-Atmosphere Cost!

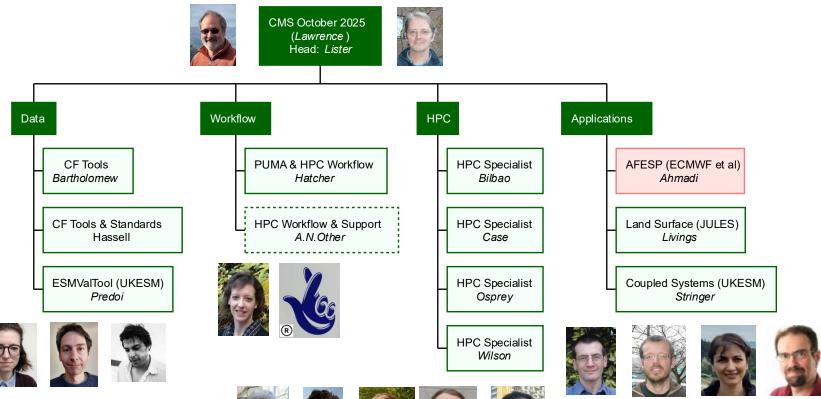
Resolution	Data	Speed (SYPD)	Nodes	Cost (NHSY)	Typical Use Case
Atmosphere: N96 ~133 km Ocean: O1 ~ 100 km	Simulation: ~0.1->0.5 TB/D JASMIN: O(PB)S	5-10	5-10	10-50	Coupled centennial climate. CMIP6, CMIP7. Physical climate and Earth System (UKESM) configurations
Atmosphere: N216 ~60 km Ocean: O25 ~ 25 km	Simulation: ~4 TB/D JASMIN: o(PB)s	2	32	384	Large Ensembles (CANARI, 6000 years!).
Atmosphere: N512 ~25 km Ocean: O12 ~ 10 km	Simulation: ~2.5 TB/D JASMIN: O(10^2TB)s O(10)PBs	0.6	80	3120	Coupled simulations, selected model intercomparison projects: HIRESMIP, EPOC. Trying to port to Grace-Hopper
Atmosphere: N1280 ~10km Ocean: 012 ~ 10 km	Simulation: ~10 TB/D? JASMIN: TBD	0.5	150	7200	Building this now, aiming to use for high resolution climate, extremes, cyclones etc.

₩ keading





NCAS Computational Model Services





















National Centre for Atmospheric Science

About





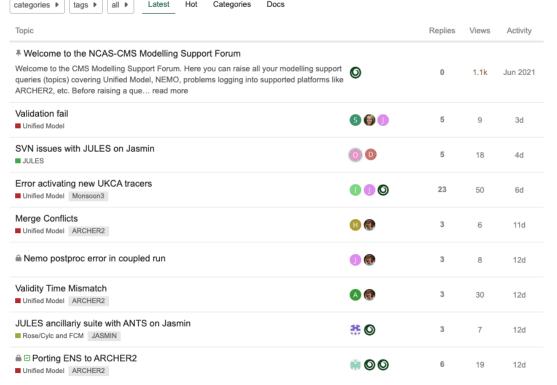


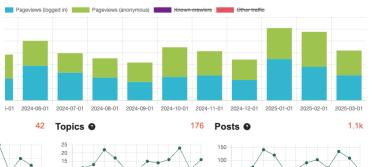
CMS Help Desk



Supporting "N02 Consortium" on ARCHER2 (and other) HPC platforms.

Year 28 MAR 2024 - 28 MAR 2025 ▼ \$









N Atl-Arctic

Ocean-Ice

N640 High Resolution

N216 Large

Ensemble

2.2km

European

CANARI: Climate Change in the Arctic-North Atlantic

Region and Impacts on the UK

(CMIP6: 500-year picontrol experiment)

WP1 Simulations

1. Run 8 "macro" historical experiments from differing initial ocean states for 1850-1950.

2. Make 5 perturbations of the 1950 atmospheric state.

3. Continue 40 historical simulations from 1950 to 2014, and

4. Continue 40 future simulations onward to 2100 using SSP370.



Domains for nested 12km and 2.2km models (Chan et al. 2020)



300

extreme

storm

cases

CANARI Large

Ensemble











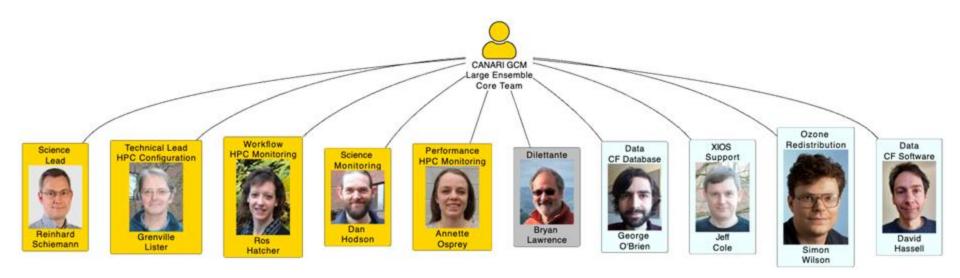


1.5km Sea

Shelf



CANARI: 6000 years of simulation Large team put the model and workflow into place

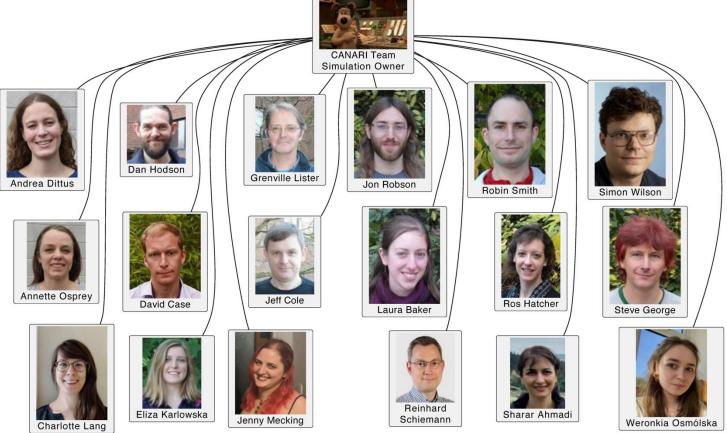


Every one of whom had/has a role to play in setting up and/or sustaining the large-ensemble.





CANARI: Large team involved in running the model







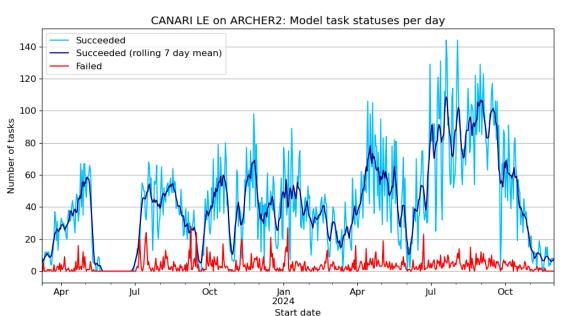
Reported Average Speeds are Misleading

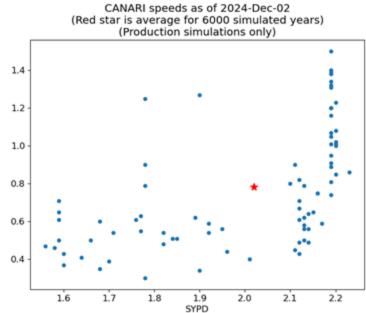






Each dot is one simulation cycle. One cycle is 3 months There were 24,000 cycles (6000 x 3-month jobs)! Most happily resubmit ... but many do not





Large Ensemble Data

Simulations

- 40 x 74 years Historical
- 40 x 76 years Future

That is:

- 40 x 150 years (1950-2100), or
- 6000 years of simulation

Output

- 822 "atomic" datasets per atmospheric simulation.
- UM boundary conditions ("frames") for several regions.
- Restart dumps monthly plus extra for "specially identified storms".
- Additional variables to support all CORDEX regions.

Data

Volumes (compressed): ~5.5 PB

- 2 PB atmos fields
- 0.5 PB atmos restarts
- 0.4 PB ocean fields
- 0.1 PB ocean restarts
- 0.1PB ice fields and restarts
- 2.1 PB of frames etc

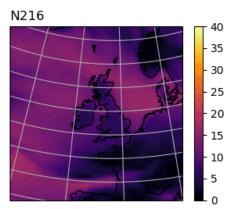
4.5 Million Files!

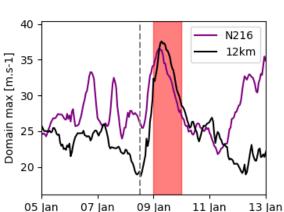
1 PB Disk used as "tape cache"

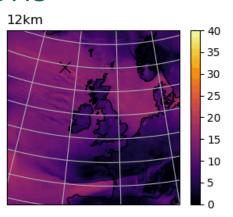
CANARI also involves nested simulations

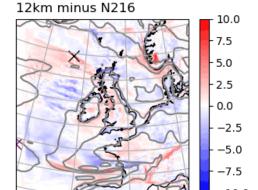
- Find the most intense windstorms in the CANARI data, and then re-simulate using nested even higher resolution model.
- The most intense UK windstorm in 2,600 years of LE data simulation
- Cold conveyor belt is more intense and sharper in the 12km RCM than the GCM















Porting to Grace-Hopper











Each node:

 Four "Super-Chips", each with a Grace CPU and a Hopper GPU.

Can we get a coupled model running on this platform?





Grace-Hopper: Why, What, and How?



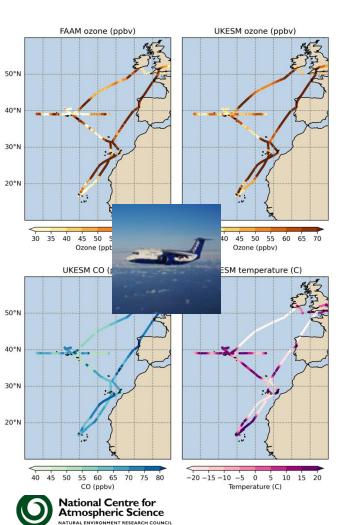
We think N512O12 might fit on this machine and run at around 2SYPD at 384 NHSY if

- We can get N512 UM atmosphere running on 64 Grace chips of 16 nodes, while
- 2. The O12 NEMO Ocean is running on the 64 Hopper GPUs, and
- 3. If we can fit all the required memory on the 16 nodes, and
- We can make a coupled model with the right version of NEMO, so that we can use
- 5. a good GPU port of NEMO via PSyclone from NG-ARCH, and
- 6. We can sort out the XIOS issues on this architecture, and finally:
- 7. We can find the necessary effort (likely ~ 4 FTE for ~6 months at least).

Much faster and cheaper than CPU version: could consider a large ensemble at this resolution which we could use for training AI systems and ...







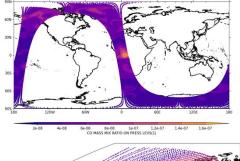


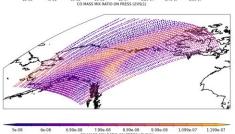


Yusuf Hamied Department of Chemistry

VISION: towards seamless integration of Model, Satellite, and In-Situ Observation

- Reduce NERC carbon data emissions by optimising impact and outcomes from the FAAM Airborne Laboratory.
- Improve policy decision making for climate mitigation by providing tools for integrating right-time observational data into Earth System Models.









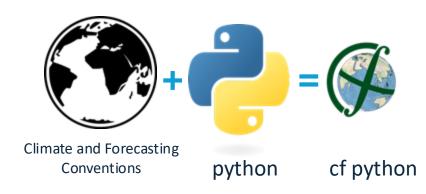


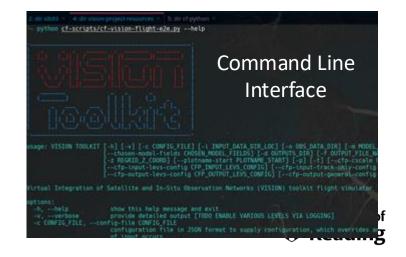


VISION toolkit: interoperable and stable software

- an accessible package that is easy and fast to use, and is portable so can be used by anyone, with any CF-compliant model and observational dataset.
- Written in python with cf-python and cf-plot, data analysis and visualisation libraries developed and maintained within NCAS.
- An important aspect of portability is that the software relies on standardised CF-compliant data from/for the models. We will provide CFnetCDF usage guidance to define what this entails.









pyfive.readthedocs.io







Traditionally, accessing HDF5 and NetCDF4 data across networks has been slower than it needs to be for three reasons:

- (1) The c-libraries (used by Python and others) which access the data are not thread-safe,
- (2) The indexes of chunk locations kept in "btrees" within the files are potentially distributed through the file, and
- (3) The chunking is often inappropriate.
- h5netcf and xarray
 support underway
- already in cf-python

No longer a *need* to use zarr or kerchunk to access data on object stores

But there are now solutions

- (1) We found, and revitalised, a pure python HDF5 reader (pyfive). It is thread-safe, and NCAS-CMS are committed to maintaining it.
- (2) The **h5repack** tool can put all the indexes at the front (but either way pyfive can access these efficiently enough).
- (3) This can often be fixed at source, otherwise, use **h5repack**!

Integral to another new tool:
PyActiveStorage, providing
remote reductions on HDF5 data.



Bonus: from a curation point of view, we are no longer dependent on a private US company to read our data in the future!



Take Home

- Climate Science can use all the available computing, and there are good scientific reasons to continue to grow our use of HPC.
 - (I haven't said anything much about Weather as we don't have time to discuss all the Al implications.)
 - (For climate science, the implications of AI are not as earth shattering as they are for weather. That's the topic of another talk.)
- But this leads to problems:
 - Our models need porting an optimizing.
 - The workflows are complex and need support.
 - Big teams are necessary to do big science. (But there can be, and are in this case, hundreds of downstream users.)
 - The data volumes and tools are challenging. Importance of standards and shared libraries.
 - Even basics like our interfaces to well established data formats need continual maintenance.
- CMS has been around for a couple of decades and continues to support the UK academic weather and climate modelling community.





That's all folks!

CMS is supported by:

- NCAS National Capability
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- The University of Reading
 With grant and project funding from
- The European Commission
 - ESIWACE Series
 - IS-ENES Series
 - ... more to come
- The Met Office
- UKRI

