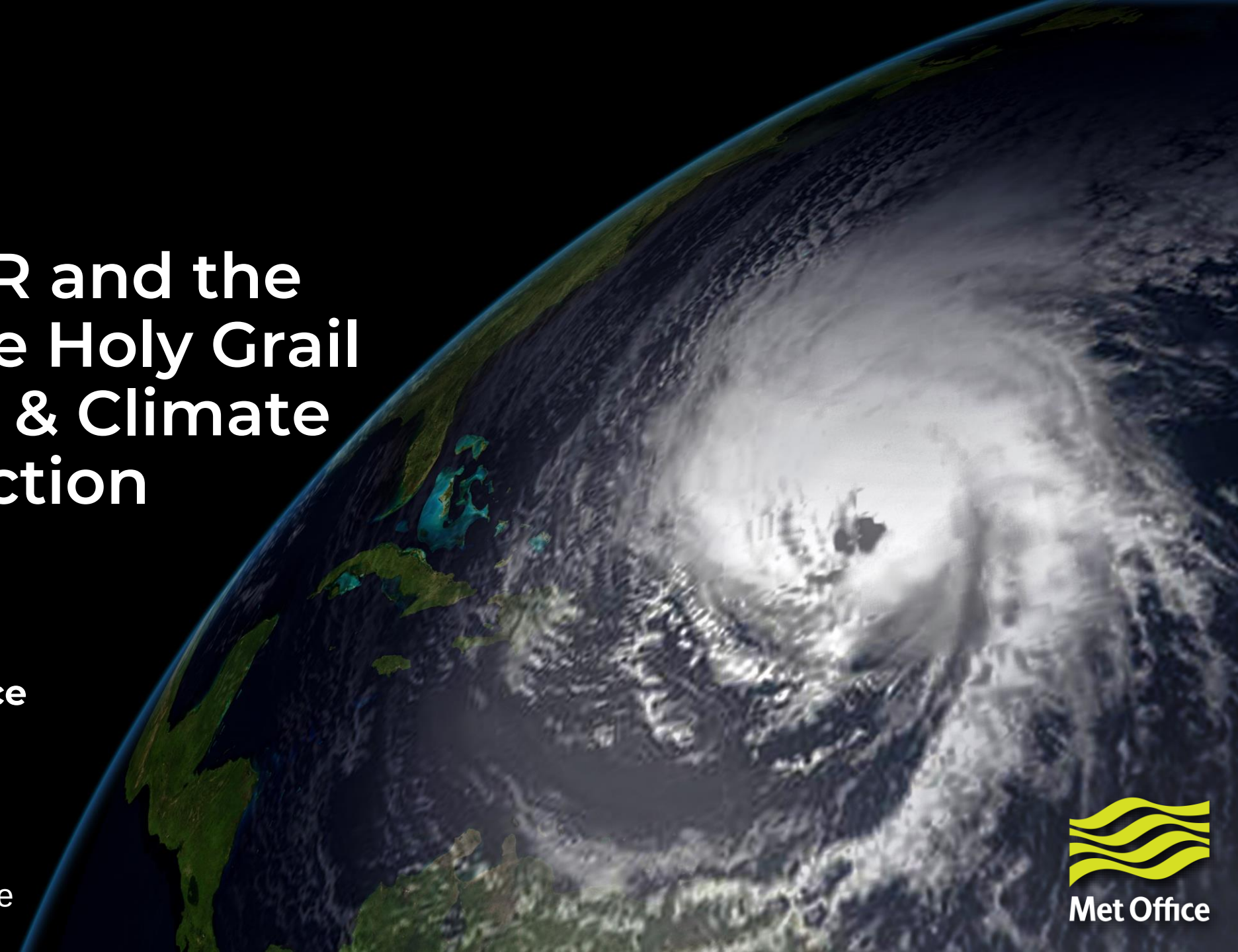
ExCALIBUR and the Quest for the Holy Grail of Weather & Climate Prediction



Nigel Wood, Met Office

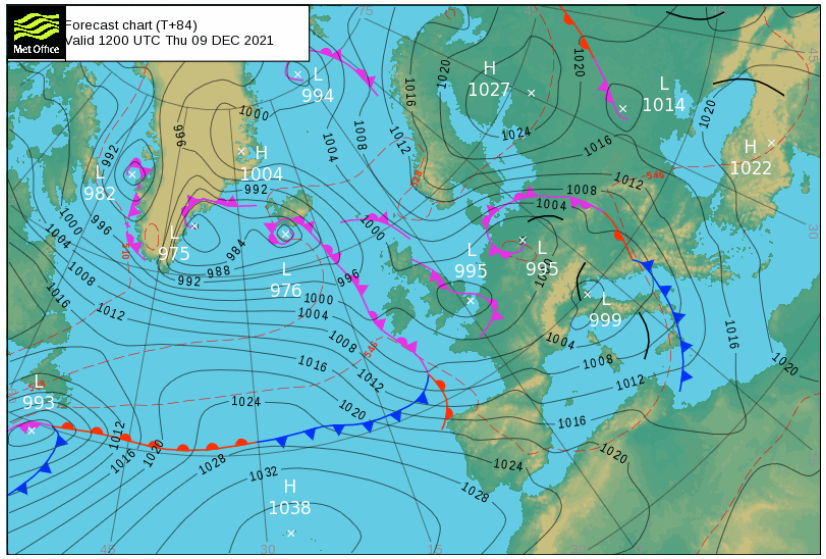
December 2021

UK's Weather & Climate prediction system

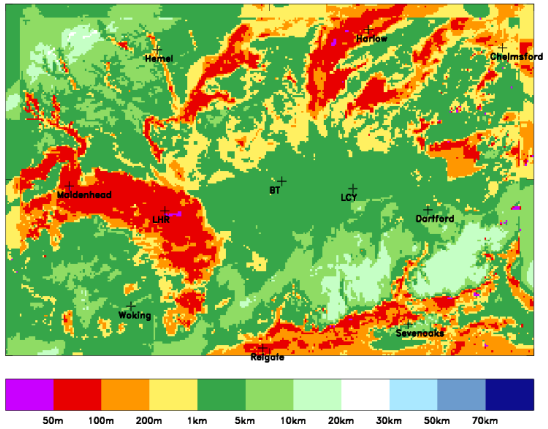
The challenge of a unified approach

- Operational forecasts
  - ➢Global (resolution approx. 10km)
  - ➢Regional (resolution approx. 1.5km)

10 km



300 m

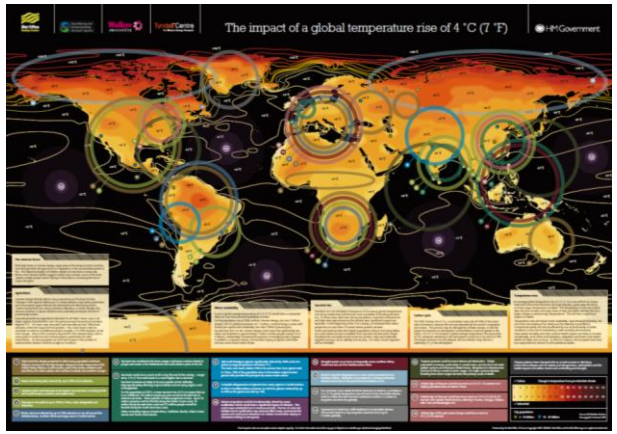


- Seasonal predictions
  - ➢Resolution approx. 60km

Unified ⇒ Same solver, same parametrisations, same code base for all

- Global and regional climate predictions
  - ➢Global resolution around 120km
  - ➢Regional around 4-1.5km
  - ➢Run for 10-100-… years

300 km

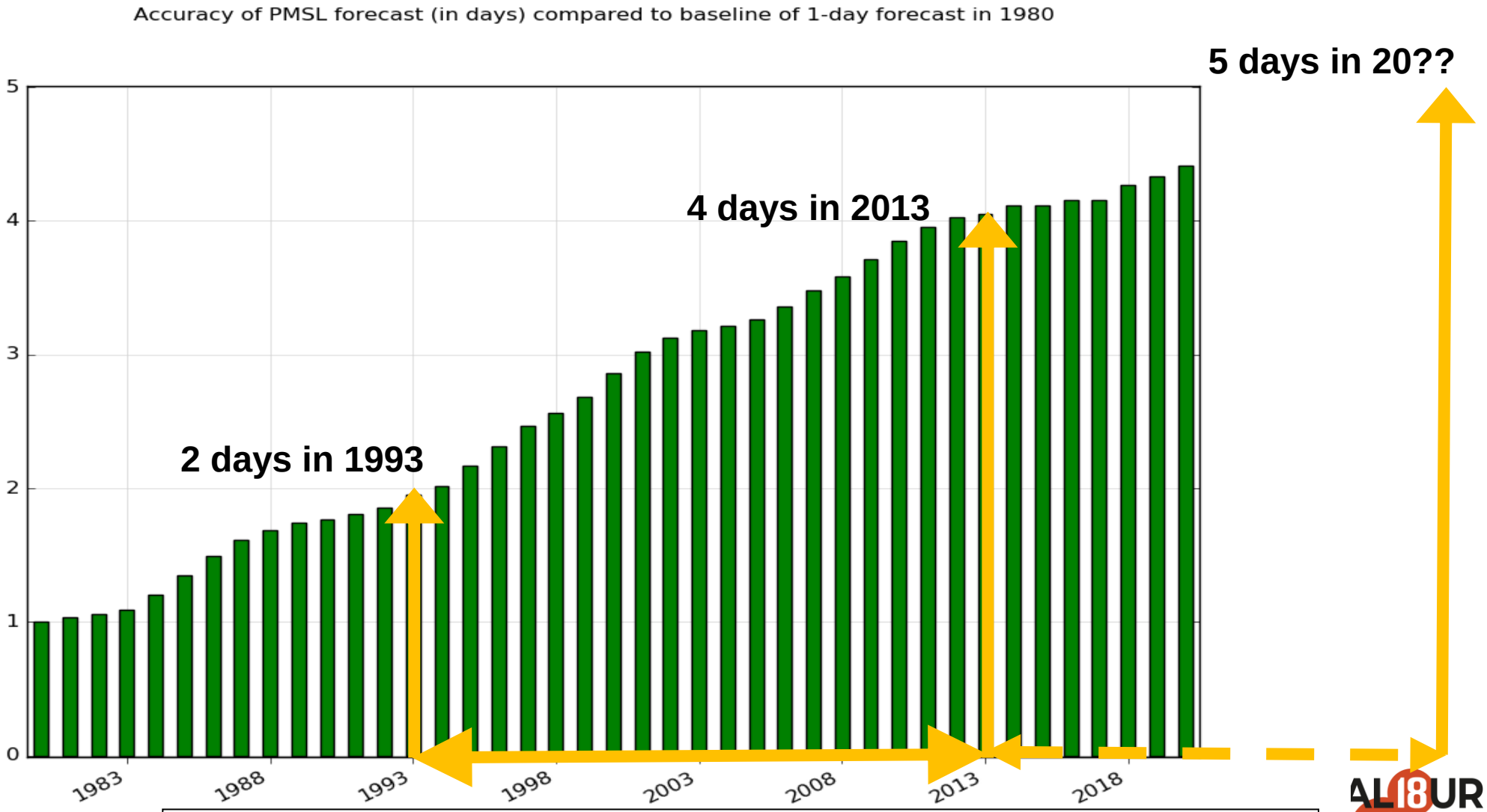


“The quiet revolution”*: ≈ 1 day’s lead time per decade

108 hour forecast today is as accurate as the 24 hour forecast was in 1980

Met Office

“…impact of Numerical Weather Prediction among greatest of any area of science… comparable to simulation of human brain and evolution of early universe”*



*Bauer, Thorpe, Brunet (2015) Nature

How do we achieve this?

What is the holy grail?

Our challenge

Why Exascale?

- Currently we simulate the world's weather at 10 km intervals
- To complete the 7 day forecast in 1 hour needs a petascale machine (16 Pflops) (we use 19,000 cores)

- To get to 5 km means 2x2 more cells and a 2 times smaller interval in time
  - **O(10)** increase in compute power & data
- To get to 1 km means 10x10 more cells and a 10 times smaller interval in time
  - **O(1000)** increase in compute power & data

GungHo/LFRic/PSyclone

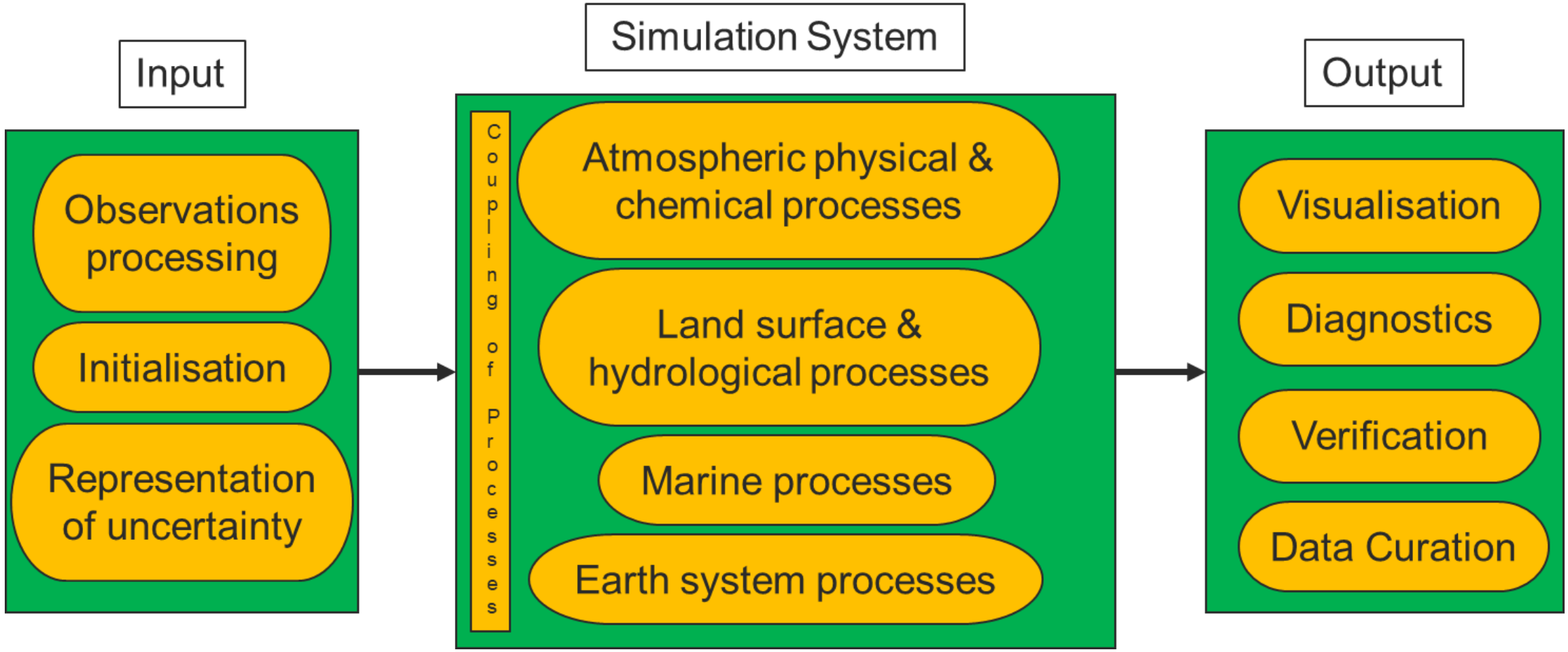
Not ExCALIBUR funded but key to delivery of next generation capability

March 2021 saw delivery of first capability of new GungHo/LFRic/PSyclone based global atmosphere model

But a lot more to do…

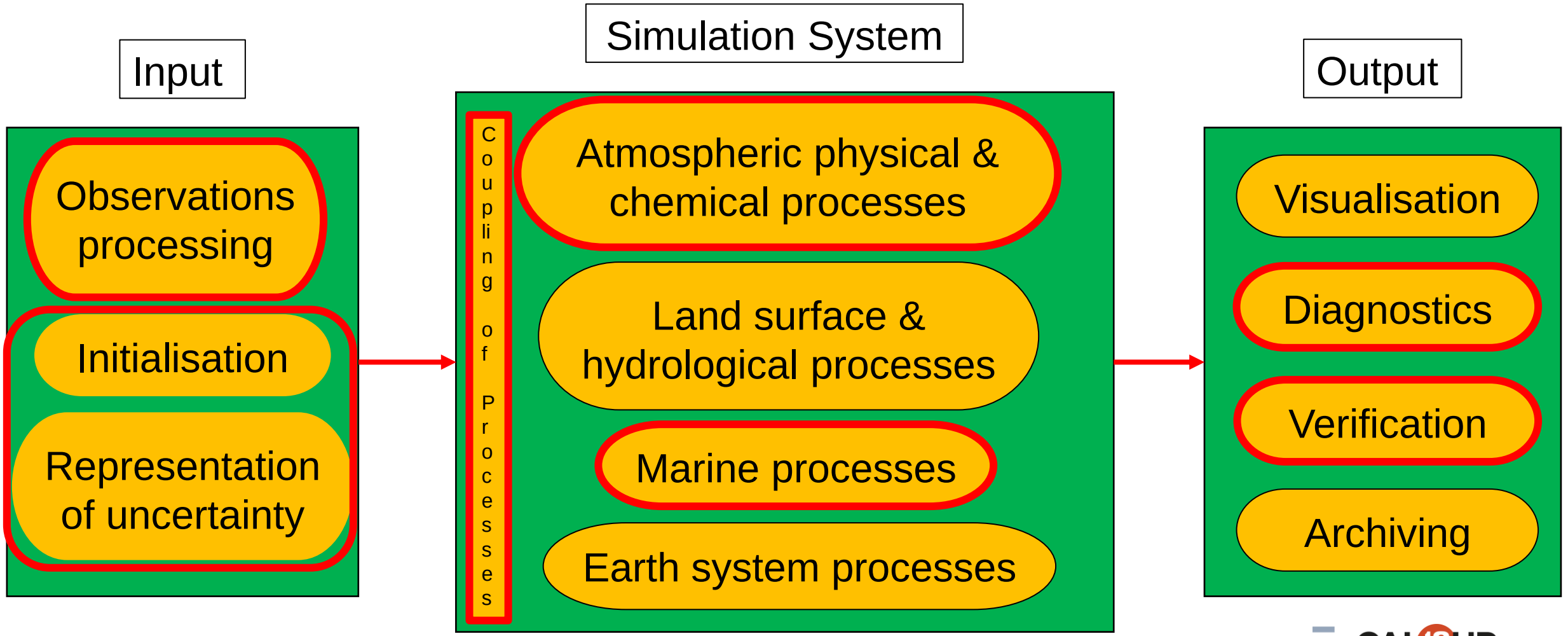
Weather & Climate prediction system

Schematic



Weather & Climate prediction system

Activities



Some example activities

Marine Systems (NEMO) design system

Delivering extension of PSyclone DSL to existing marine systems without rewriting code (fruition of GOCEAN POC)

Atmospheric Model data layout and memory access design system

Delivering mixed precision capability & flexibility in memory layout

Atmospheric observation pre-processing and assimilation

Delivering new flexible framework deployable across different architectures

Performance Portability for Existing Marine-Systems Models

NEMO

MEDUSA

NEMOVAR

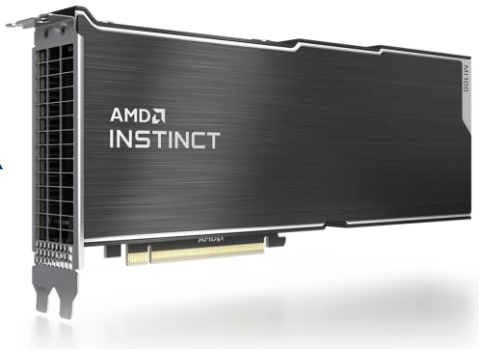
WAVEWATCH III

PSyclone

OpenMP

OpenACC

OpenMP



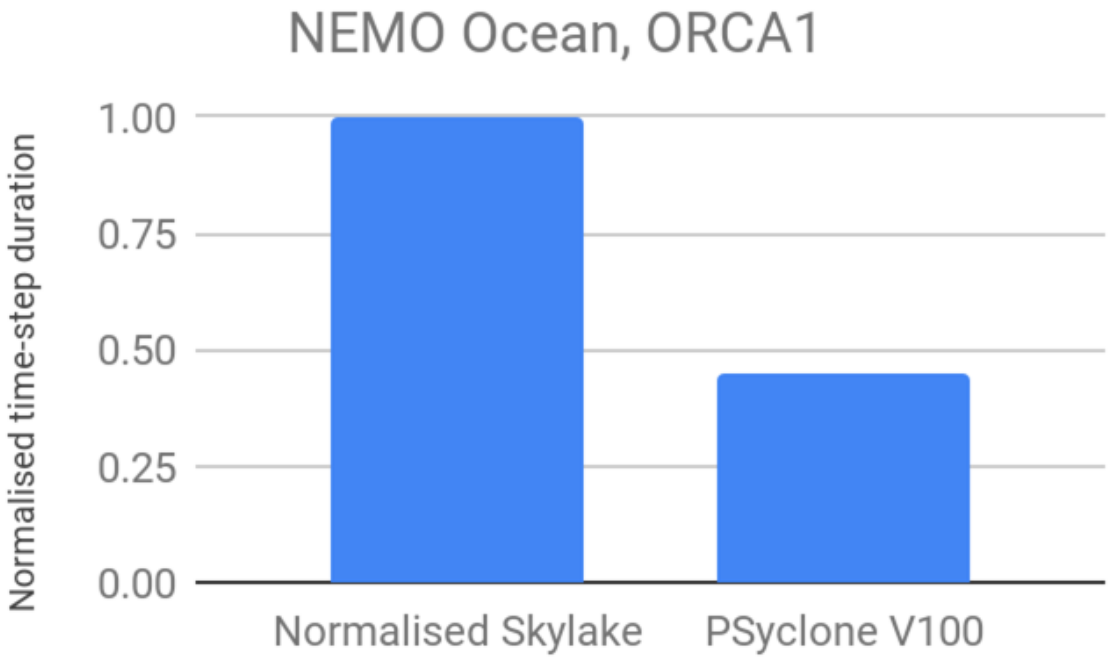
UKRI Science and Technology Facilities Council
Hartree Centre

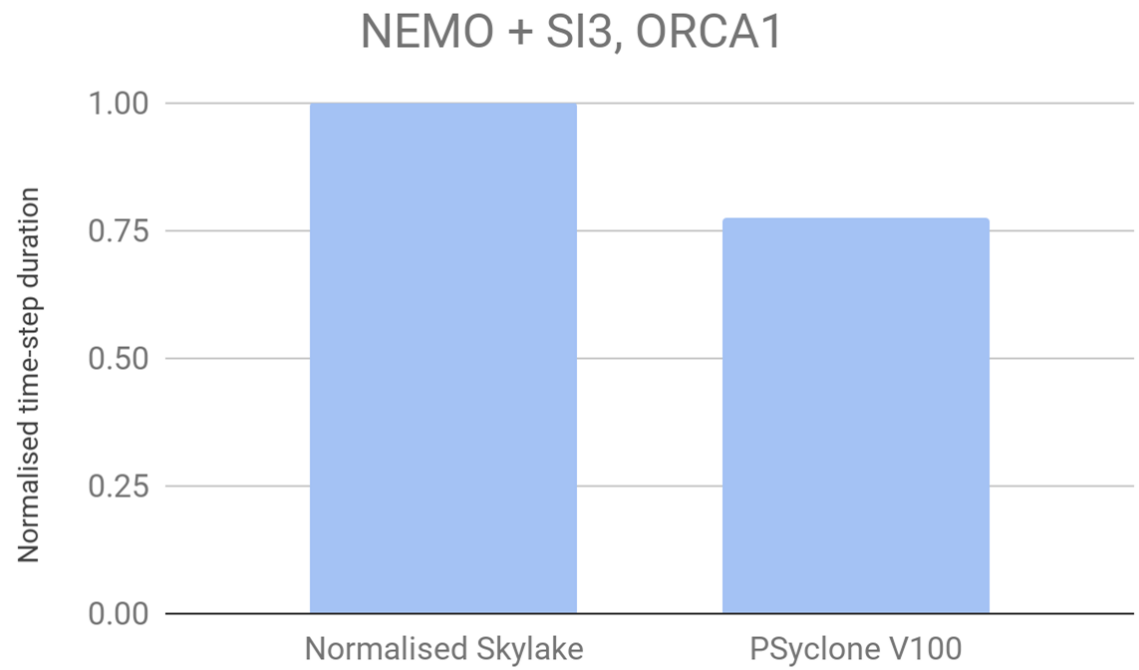
National Oceanography Centre

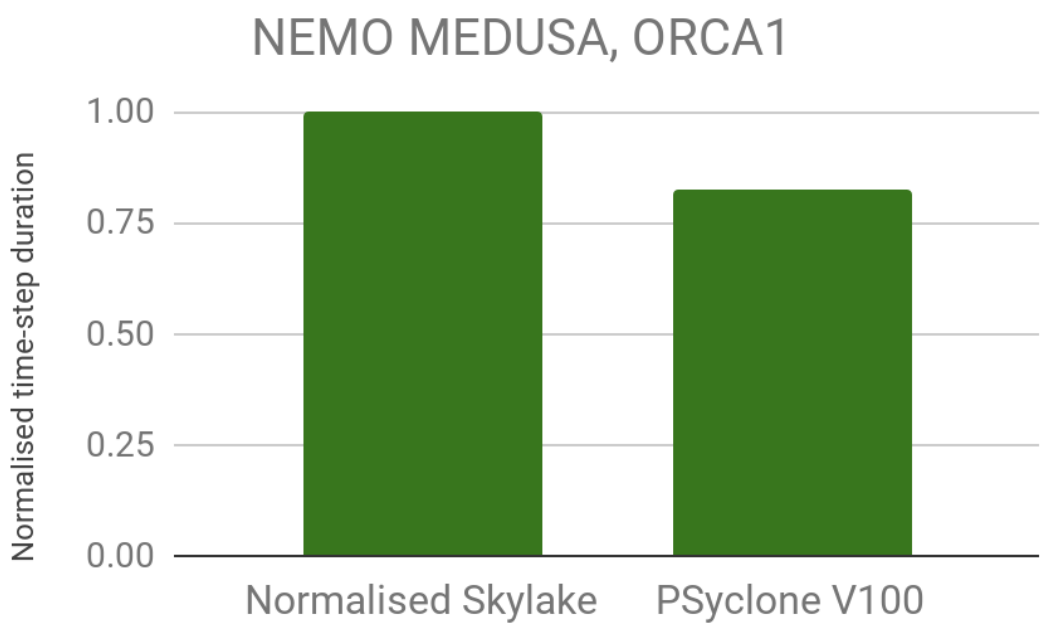
National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL

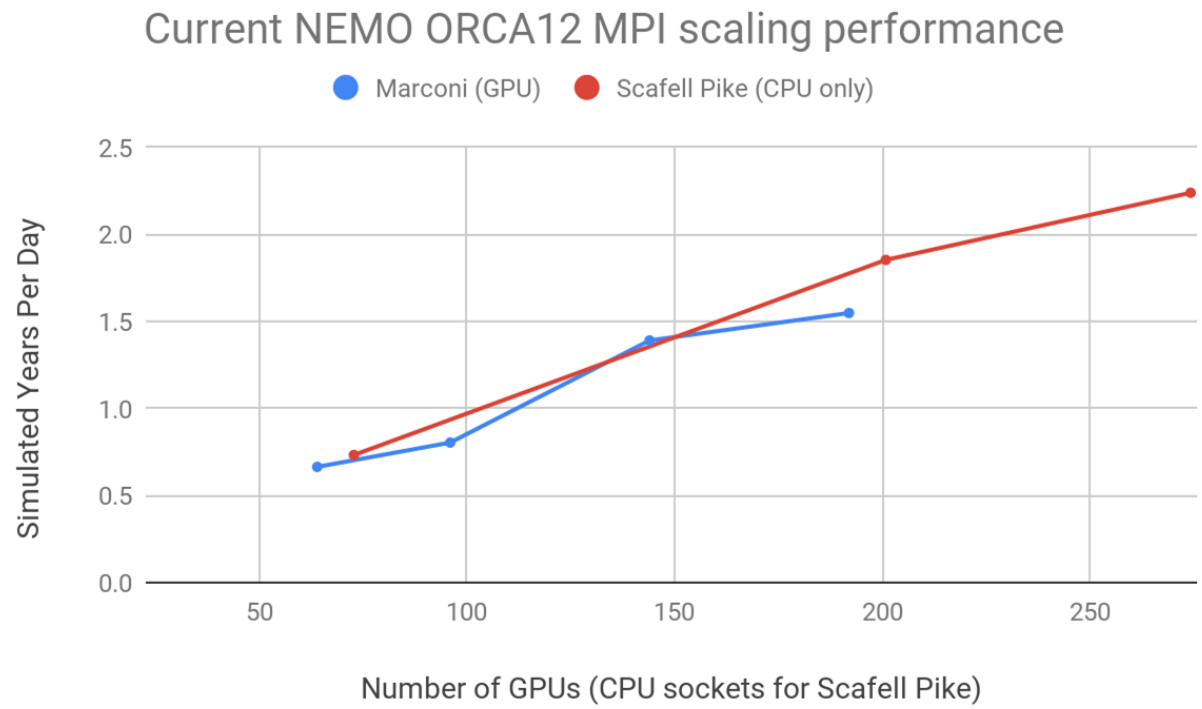
Met Office

NVIDIA

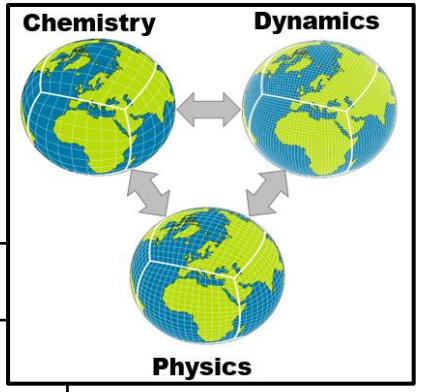

NEMO Ocean, ORCA1
Normalised time-step duration
1.00
0.75
0.50
0.25
0.00
Normalised Skylake
PSyclone V100


NEMO + SI3, ORCA1
Normalised time-step duration
1.00
0.75
0.50
0.25
0.00
Normalised Skylake
PSyclone V100

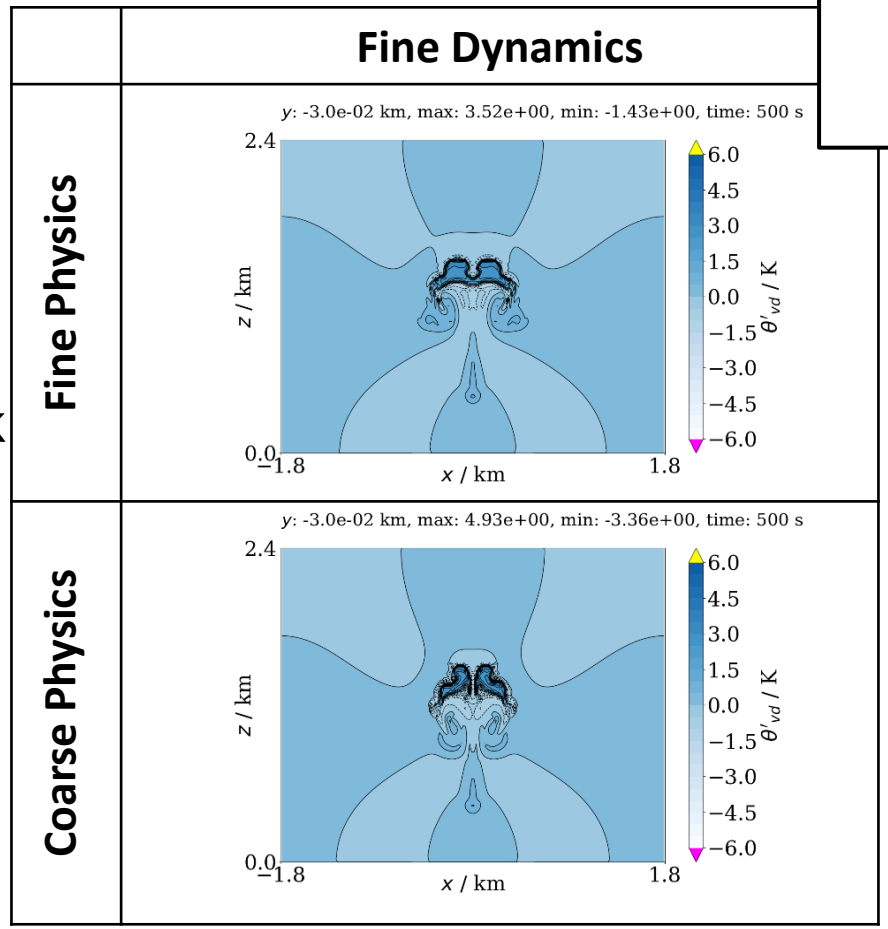

NEMO MEDUSA, ORCA1
Normalised time-step duration
1.00
0.75
0.50
0.25
0.00
Normalised Skylake
PSyclone V100


Current NEMO ORCA12 MPI scaling performance
Marconi (GPU)
Scafell Pike (CPU only)
Simulated Years Per Day
2.5
2.0
1.5
1.0
0.5
0.0
50
100
150
200
250
Number of GPUs (CPU sockets for Scafell Pike)

Atmospheric Model data layout, memory access design system, and spatial decoupling of processes



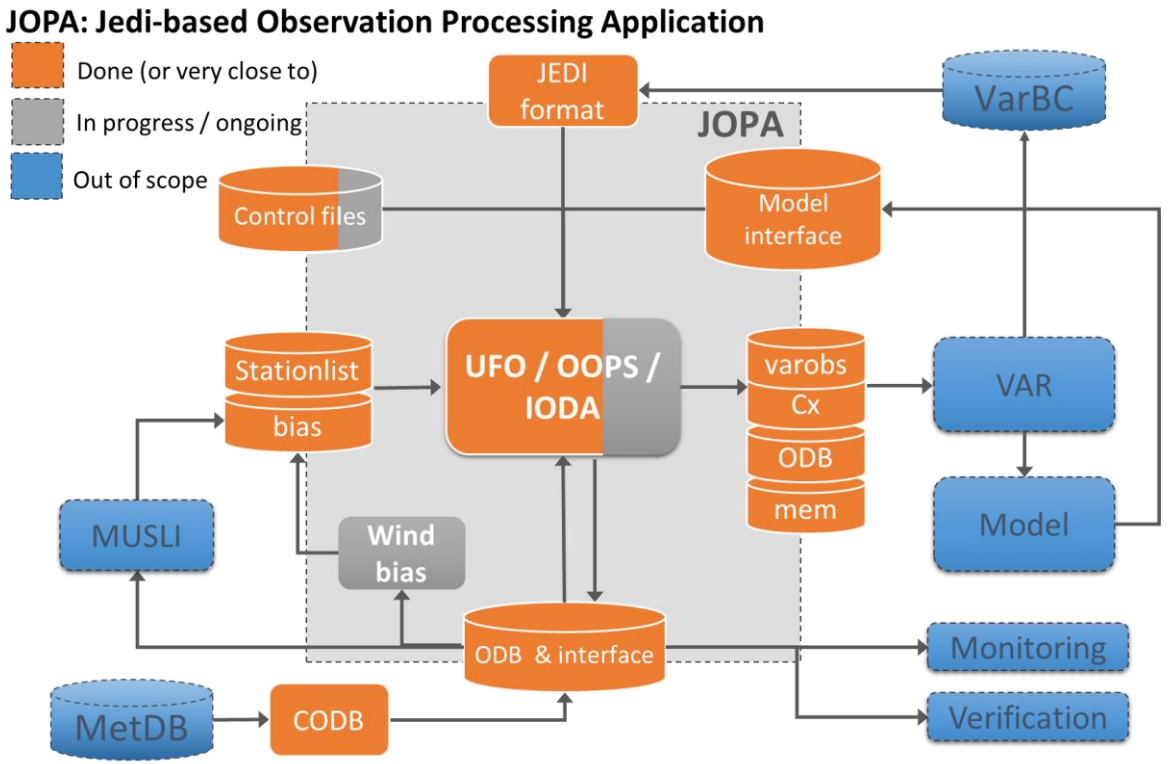
- **Only do what is needed:** Example miniapp implementation capable of spatial splitting of combinations of transport, dynamics and UM physics parametrizations.
- **Only do it to the accuracy needed:** framework in place for mixed-precision, but suspected compiler in Gnu means refactoring needed to demonstrate benefit.
- **Do it using the optimal data layout:** Implementation of the "i-first" data transpose to the microphysics code in the LFRic basic-gal model shows a **4x speed up** in that part of the model.



A moist bubble test showing the impact of running the physics (condensation/cloud scheme) at a coarser resolution.

Next-Generation observation processing

Key infrastructure developments achieved



- Automatic Schema
- Global UM interface
  (incl. background error / Rho-Theta level)
- VarObs/CX, interfaces
- Multiple UFO filters (thinning, Composite operator, where clause , etc …)
- ODB full backend to IODA
- Comparison suite
- Generic auxiliary files interface (incl. netcdf / csv)
  used by obs. error, VarBC coeff., Static bias, station list
- Improved ObsSpace Group (Derived Observation)
- Generic (& user defined) QC diagnostics flag

Cross-Cutting Activities

Software Environment for Actionable & VVUQ-evaluated Exascale Applications (SEAVEA)

UCL Brunel

ExCALIStore (IO & Storage)

Reading & Cambridge NCAS

Uncertainty Quantification at the Exascale (EXA-UQ)

Exeter

ExCALIWork (Workflow)

Reading NCAS; StackHPC; DDN

Efficient Cross-Domain DSL Development for Exascale

Edinburgh
Imperial College London

Task parallelism

Durham & STFC Hartree

I/O Infrastructure investigations

Met Office

Advanced Parallel in Time Algorithms for Partial Differential Equations (**APinTA PDEs**)

Exeter & Imperial

Workflow Design and Analysis

Met Office

Containers

Met Office

SiMLInt *(sim-el-int)*, Simulation and Machine Learning Integration

EPCC

Thank you! Questions?

See https://excalibur.ac.uk/ for more