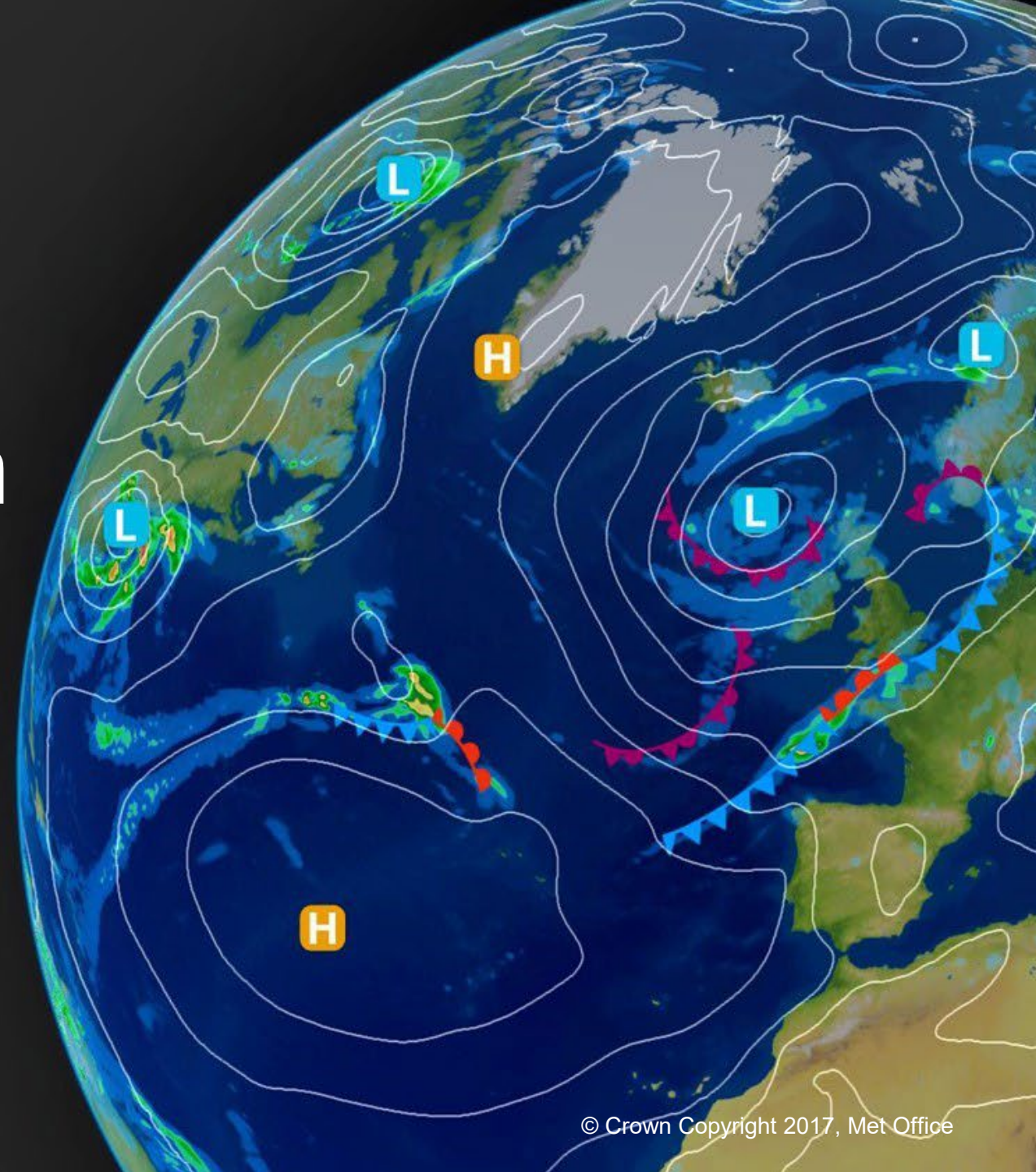


# LFRic and NGMS: Meeting challenges of exascale through diversifying HPC

Iva Kavčič, Met Office, UK

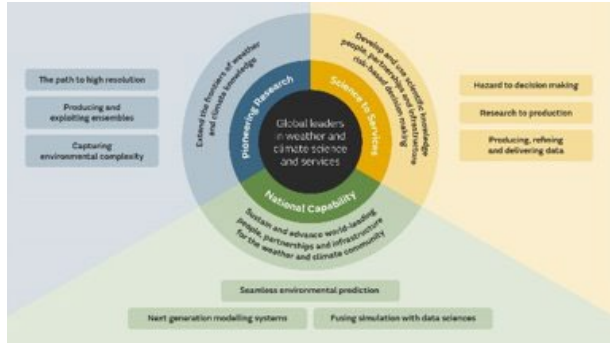
+ *many others!*

20th ECMWF workshop on high performance  
computing in meteorology, 10 October 2023



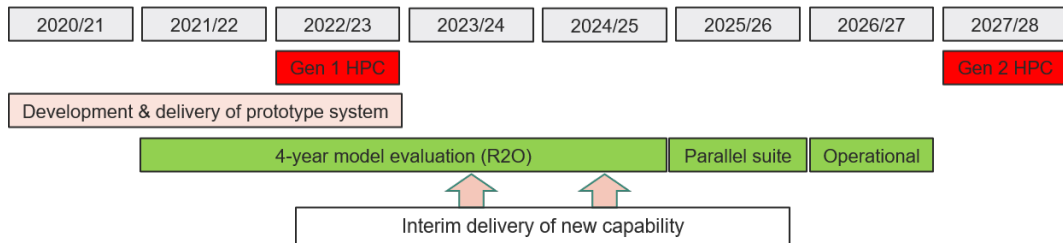
# Met Office Next Generation Modelling Systems (NGMS) Programme

## NGMS Programme vision

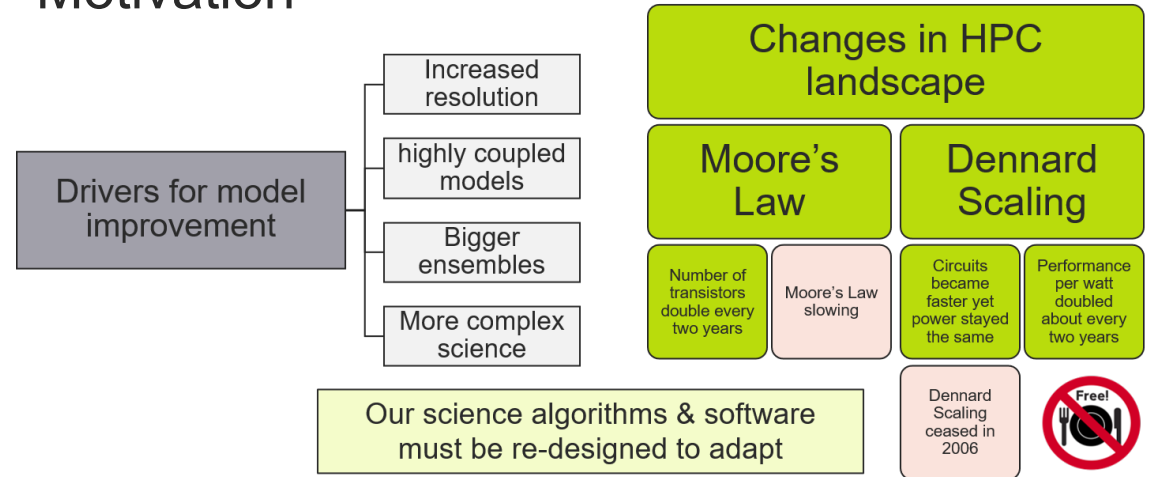


***“To reformulate and redesign our complete weather and climate research and operational/production systems, including oceans and the environment, to allow the Met Office and its partners to fully exploit future generations of supercomputer for the benefits of society.”***

## A reminder of timescales



## Motivation



## NGMS Benefits



Improved scalability



Exploit new HPC

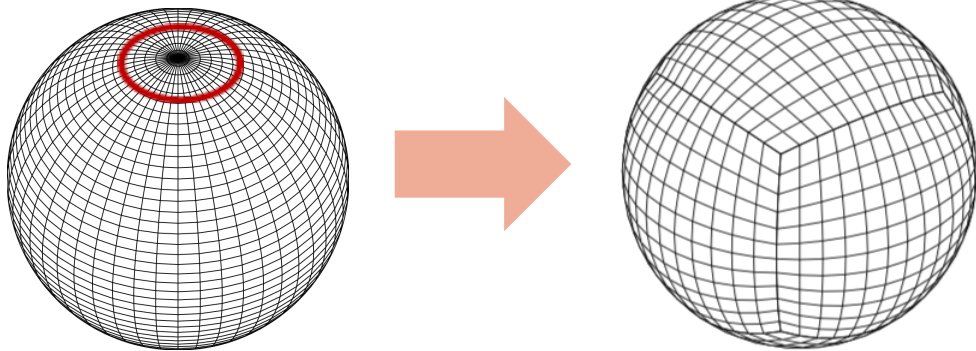


Grow external collaborations



Enable new science

# Atmosphere modelling system: GungHo dynamical core + LFRic Software Infrastructure + Separation of Concerns



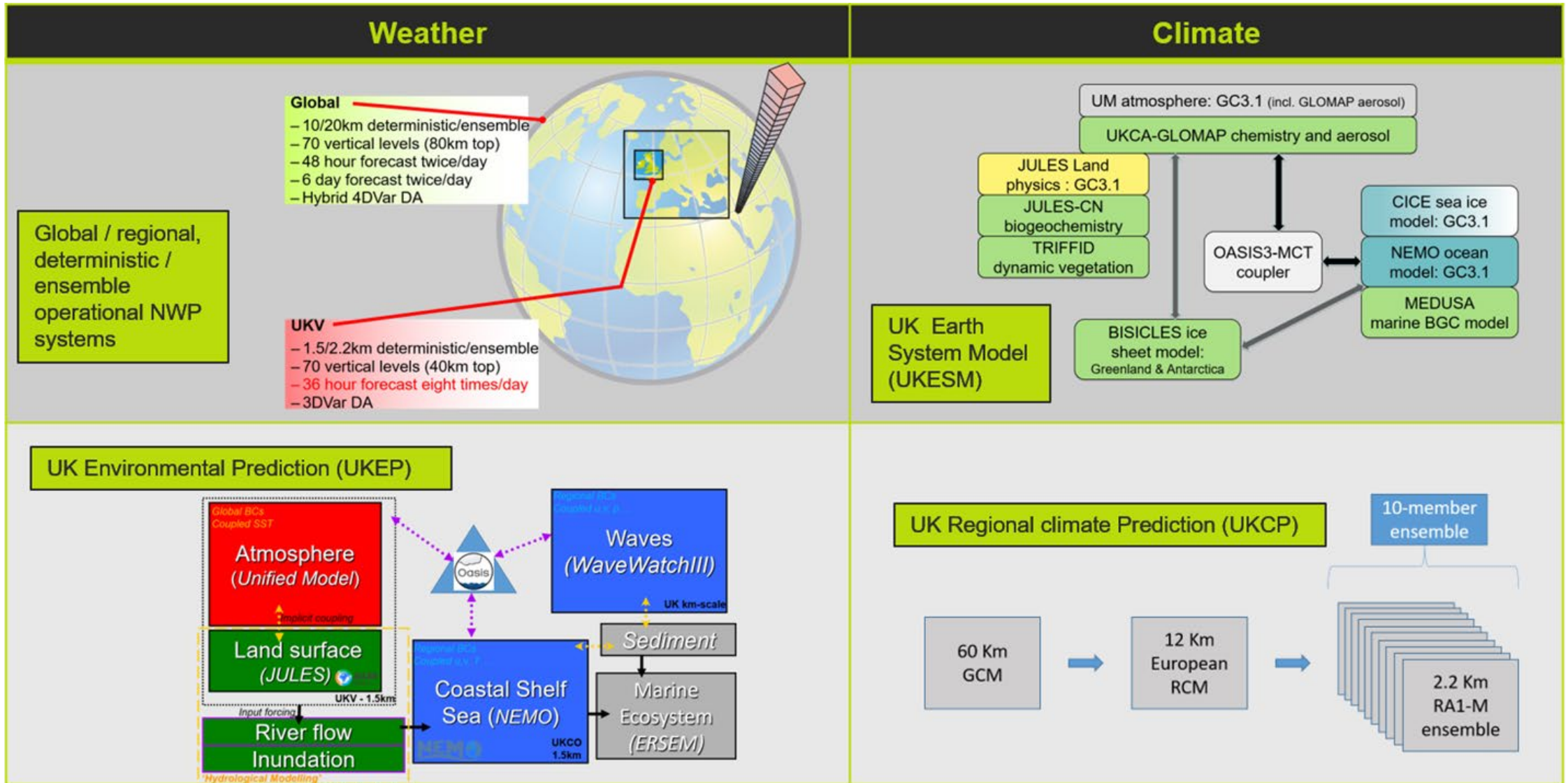
**Unified Model**

**LFRic**

1. Increased **resolution**
2. New dynamical core (**mesh** and spatial **discretisation**)
3. Performance **portability**

1. → Exascale **computation (DSLs)** and high volume of **data (I/O)**.
2. → New data **structures** and **layout (regridding; coupling; compiler support)**.
3. → New **architectures** (deployment of **software stack**).

# Met Office Programme scope – *what we have to consider*



### Observations

- JOPA obs processing (JEDI)
- JADA data assimilation (JEDI)
- NEMOVar
- LIS (land surface)

### Atmosphere components

- GungHo dynamical core
- UM Physics
- UKCA chemistry

### Infrastructure

- LFRic
- Rose
- Cylc
- XIOS
- ANTS
- PScyclone
- YAXT

### Marine systems

- NEMO Ocean
- NEMO Sea Ice SI3
- MEDUSA& ERSEM biogeochemistry
- WaveWatch III wave model

### Coupler

- OASIS
- ESMF

### Verification

- MET
- TRUI
- ESMValTools

### Land systems

- HydroJULES land model
- BISICLES land ice

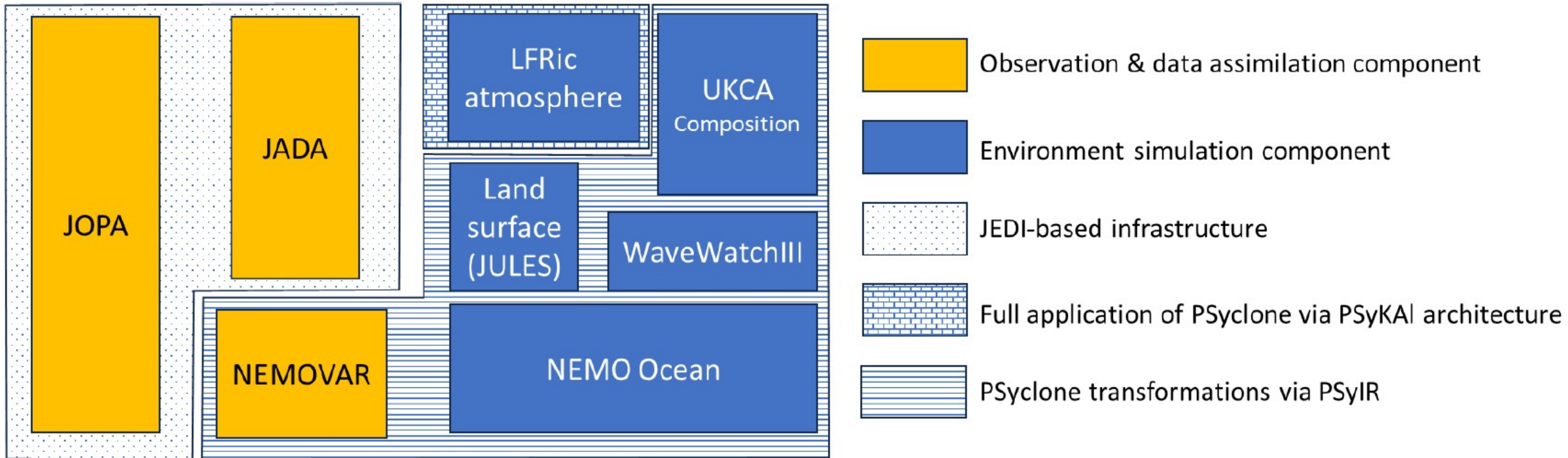
### Visualisation

- IRIS (extended)

# Managing diversity of platforms and workflows

## Separation of concerns

- ❖ Separating the science from the software framework (e.g. contributions from different institutions).
- ❖ Separating the coding of the scientific algorithms from the parallel implementation on specific architectures (e.g. domain-specific languages).



## Schematic of the main components of Momentum and their approaches to a separation of concerns (Wood et al, 2023)

*PSyKAI = Parallel System, Kernel, Algorithm; PSyIR = PSyclone Internal Representation (STFC)*

*JEDI = Joint Effort for Data assimilation Integration (JCSDA)*

**PSyclone** (“PSy” + “clone”) is a domain-specific compiler and source-to-source translator to provide performance portability and separation of concerns. *(Sergi Siso’s talk on Friday 13th October)*

- A tool to record and apply the **knowledge of HPC experts**: optimisations encoded as a ‘recipe’ (scripts) rather than baked into the scientific source code.
- Different recipes for different computer architectures (CPU, GPU); Supports **distributed** and **shared-memory** parallelism.
- **Used in all main aspects of Momentum™ Framework**: Atmosphere modelling system (LFRic), Marine modelling system (NEMO), Data Assimilation (PSyAD = “PSyclone ADjoint”, adjoint code generation).





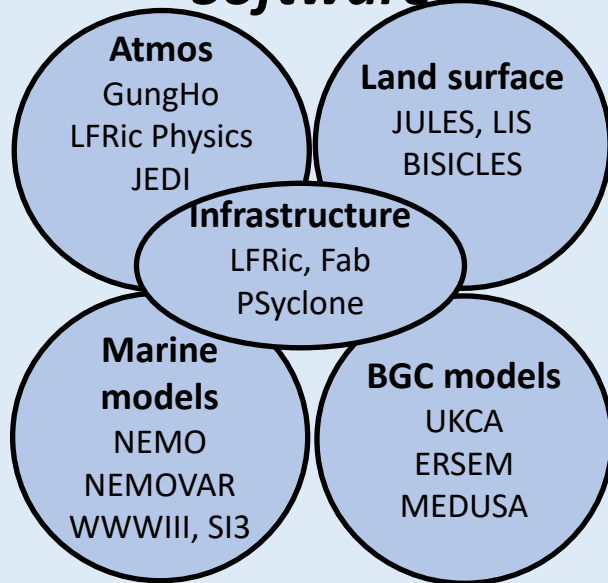
**Momentum**<sup>TM</sup>

The Unified Earth Environment  
Prediction Framework

# The Momentum™ Partnership

## Momentum™: The Unified Earth Environment Prediction Framework

### Software



### Science Configurations

GC: GAL, GOSI and RC: RAL, CO  
JOPA & JADA

MOGREPS

GLOSEA

UKESM

ACCESS

NCUM

GALWEM

NZESM

### Prediction Systems

**Software** comprising the model codes and supporting infrastructure *provides the ability to run regional and global applications*

**Science Configurations** *define the way model codes are run for regional or global applications*

**Prediction Systems** *enable delivery of forecasts and predictions*

# NGMS project status – October 2023

green=active; purple=closed; blue=ExCALIBUR-resourced

## NG-UX

- Julia Cantarano [George Pankiewicz]
- Develop and inaugural delivery of NGMS training material transitioning to BaU. This project will include aspects of usability

## GungHo Atmosphere Science Project

Ben Shipway [Nigel Wood]

- Develop atmospheric science aspects & deliver model scientifically as good as UM

## LFRic Infrastructure Development

Steve Mullerworth

[JC Rioual]

- Deliver infrastructure to replace the UM scalable for future platforms

## LFRic Inputs

Iva Kavčič [JC Rioual]

- Tools to ingest fixed & time-varying fields.
- Include initial conditions, ancillary fields and LBCs

## NG-VAT

Kevin Wheeler [Glenn Greed]

- Analysis & visualisation of LFRic model data with Iris

## NG-Marine Systems

Mike Bell [Andy Saulter]

- Deliver scalable marine systems including ocean, sea-ice & wave models

## NG-Coupling

JC Rioual [Ben Shipway]

- OASIS3-MCT coupled components

## RAL3-LFRic

Mike Bush [Huw Lewis]

- Deliver LFRic-based RAL3 research configuration as a well-tested & understood baseline for future developments

## NG-PAO

David Simonin [Chiara Piccolo]

- JEDI as a DA framework
- Processing of NWP observational data for NG-DA

## GC5-LFRic

Maria Carvalho [Alistair Sellar]

- Development & evaluation of GC for Climate & NWP within LFRic framework

## FAB Build System

Rich Gilham [Glenn Greed]

- Development of new build systems for NGMS components

## NG-R2O

Mike Thurlow [David Walters]

- Support transition of NGMS capability from research to NWP operations

## NG-Composition

Fiona O'Connor [Matt Hort]

- Coordination of aerosol & chemistry development within NGMS

## NG-Ver

Phil Gill [Joanne Robbins]

- Development of NWP verification capability for NGMS

## NG-R2C

Jon Seddon [Richard Wood]

- Support transition of capability from research to climate production

## NG-Name

Ben Devenish [Matt Hort]

- Development of dispersion models (e.g. NAME) for next generation computing

## NG-Integration

- Sam Adams [JC Rioual]
- Provide a focus for IO development, cloud computing and integration

## NG-Optimisation

- Chris Maynard [JC Rioual]
- Optimisation of NGMS components with initial focus on LFRic

# Diversity of skills and people

## **Role: Scientific Software Engineer\*, Met Office**

- ❖ Recruitment
- ❖ Training
- ❖ Community

*a.k.a Research Software Engineer*

## Is Research Software Engineering coming of age?



- Neil Chue Hong
- Director of the Software Sustainability Institute

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Chue Hong, Neil (2023). Is Research Software  
Engineering coming of age?

<https://doi.org/10.6084/m9.figshare.24078054>

Picture credits available in slide notes

Has a PhD

In the sciences

Works for a  
university

In the  
sciences

Is male

Is white

## The modal RSE

Has an ORCID

Is named as a  
co-author

On a permanent  
contract

Bus factor of 1

Uses

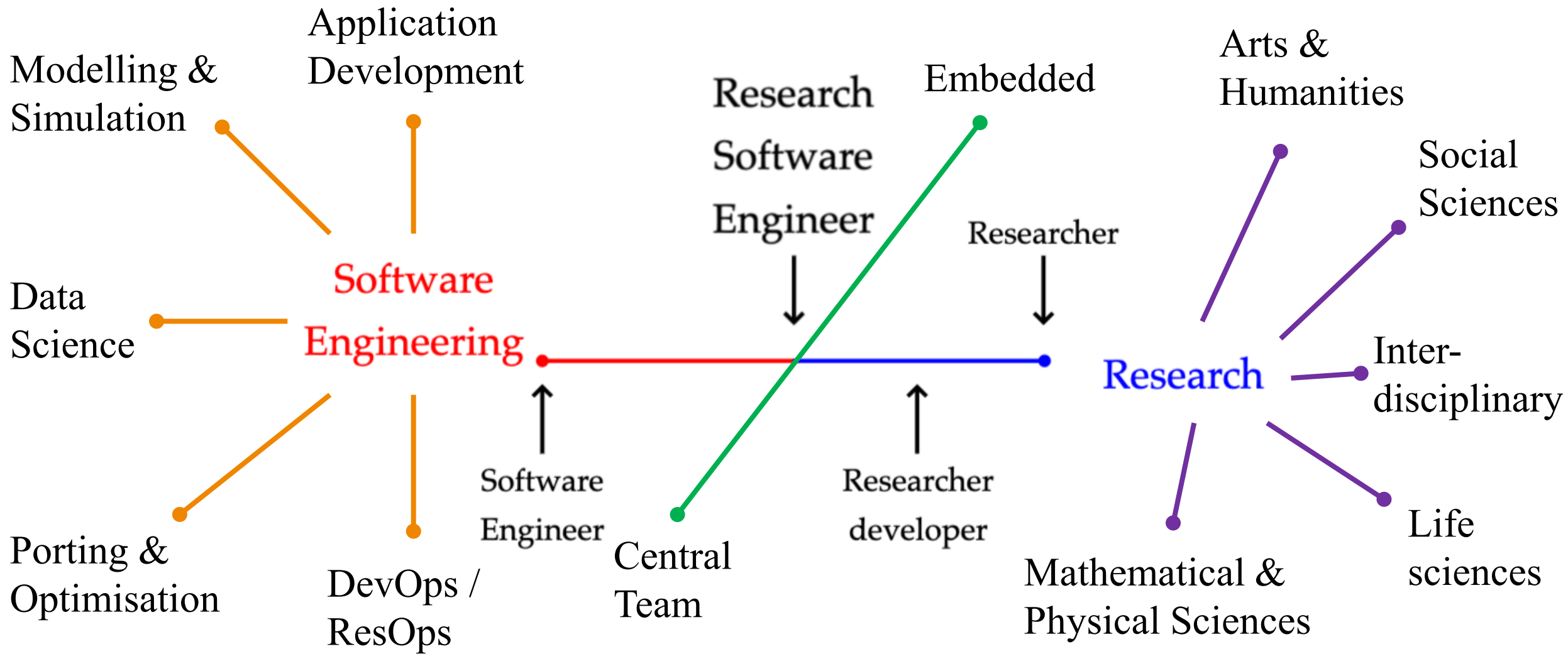
open source  
all the time

Uses Git

Uses Python

Uses GNU/Linux

Has been to an  
RSE conference





# Recruiting for diversity: Generic SSE campaign

- **SSE teams** (Science IT) and **embedded SSEs** (predominantly science teams).
- **No explicit requirement for a degree and/or language tools.**
- **Technical skills:** Interest (Foundation SSE), ability (SSE) and leadership role (Senior SSE) in developing/maintaining software applications and QA (*assessment by programming exercise and interview*).
- **Interpersonal skills:** Teamworking and communication with diverse audience, prioritising (FSSE/SSE) or/and managing work (SSE) to deliver outcomes. Desire and ability to learn and apply new skills.
- **Encourage people** who are **changing careers** or/and **returning** to workforce **after a career break**. Adjustments under **Disability Confident Scheme**.

# Training and skills development

- **SSE Induction Programme** (within 6-12 months from joining the office).
  - Training **courses** (external providers, more experienced colleagues).
  - **Work** in a new starter's main role (from simple to complex tasks).
  - Two **short projects** (often unrelated to work, working together with peers).
  - Include Industrial Placement Students and Apprentices.
  - **Feedback** from participants to improve process.
- **Placements/secondments** in other teams (usually 3 to 6 months).
- **Continuous professional development** (e.g. workshops/conferences, moving teams, projects with external partners) and **knowledge transfer**.

# Community



*Met Office SSEs at RSECon23*

- **SSE Community of Practice.**
- **Staff networks** (e.g. new starters, skills-related, general interests, EDI).
- **Mentoring** scheme.
- **Supportive working environment:** collaboration spaces and quiet spaces, arrangements for specific needs.

*A good place to develop (research) software engineering skills!*

# Questions?

## (Some) References

- Wood et al. (2023), *Seamless environmental, weather and climate predictions for Exascale era computing: building Momentum<sup>TM</sup>*, Bulletin of AMS, submitted.
- Sergeev et al. (2023), [Simulations of idealised 3D atmospheric flows on terrestrial planets using LFRic-Atmosphere](#), Geophysical Model Development, volume 16, issue 19, 5601–5626.
- Adams et al. (2019), [LFRic: Meeting the challenges of scalability and performance portability in Weather and Climate models](#), Journal of Parallel and Distributed Computing, 132, 383-396.
- PSyclone documentation: <https://psyclone.readthedocs.io>