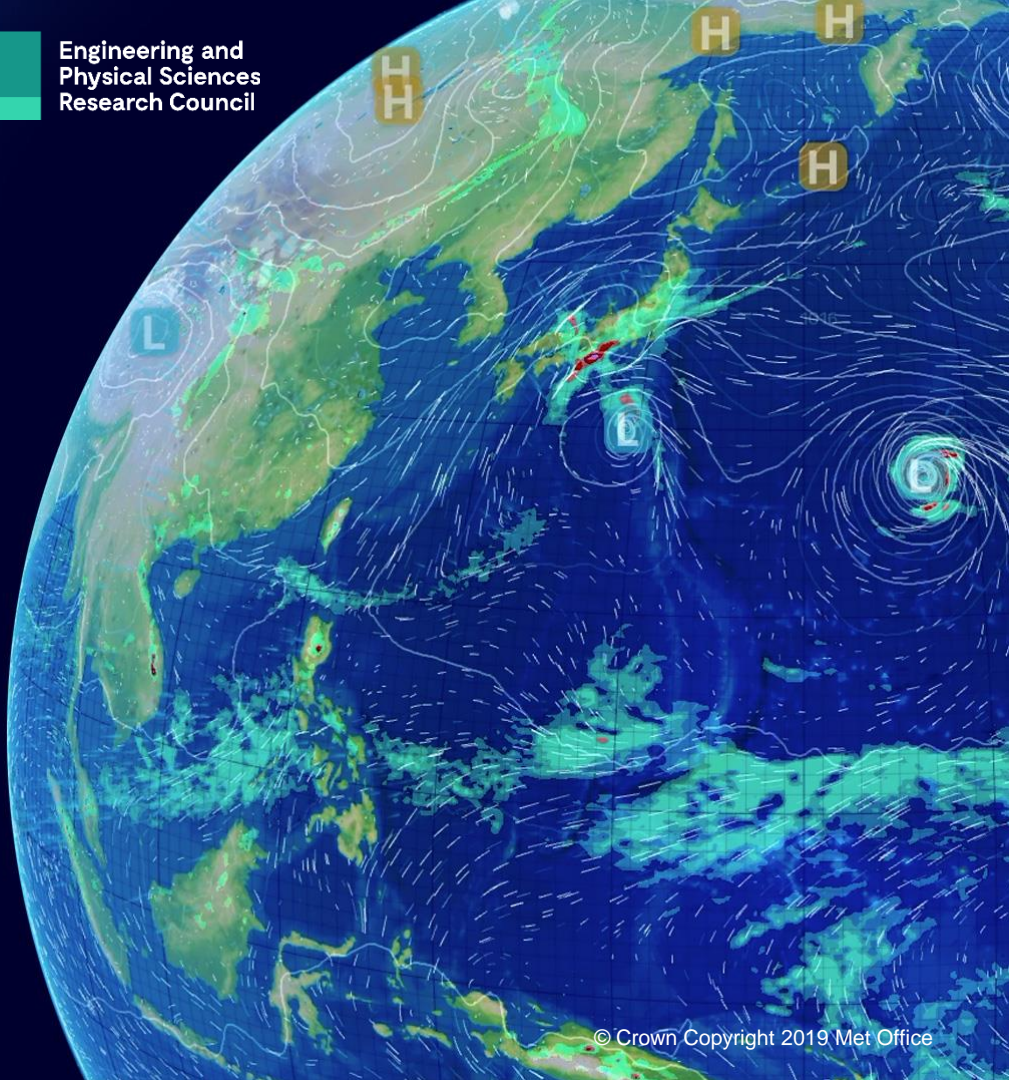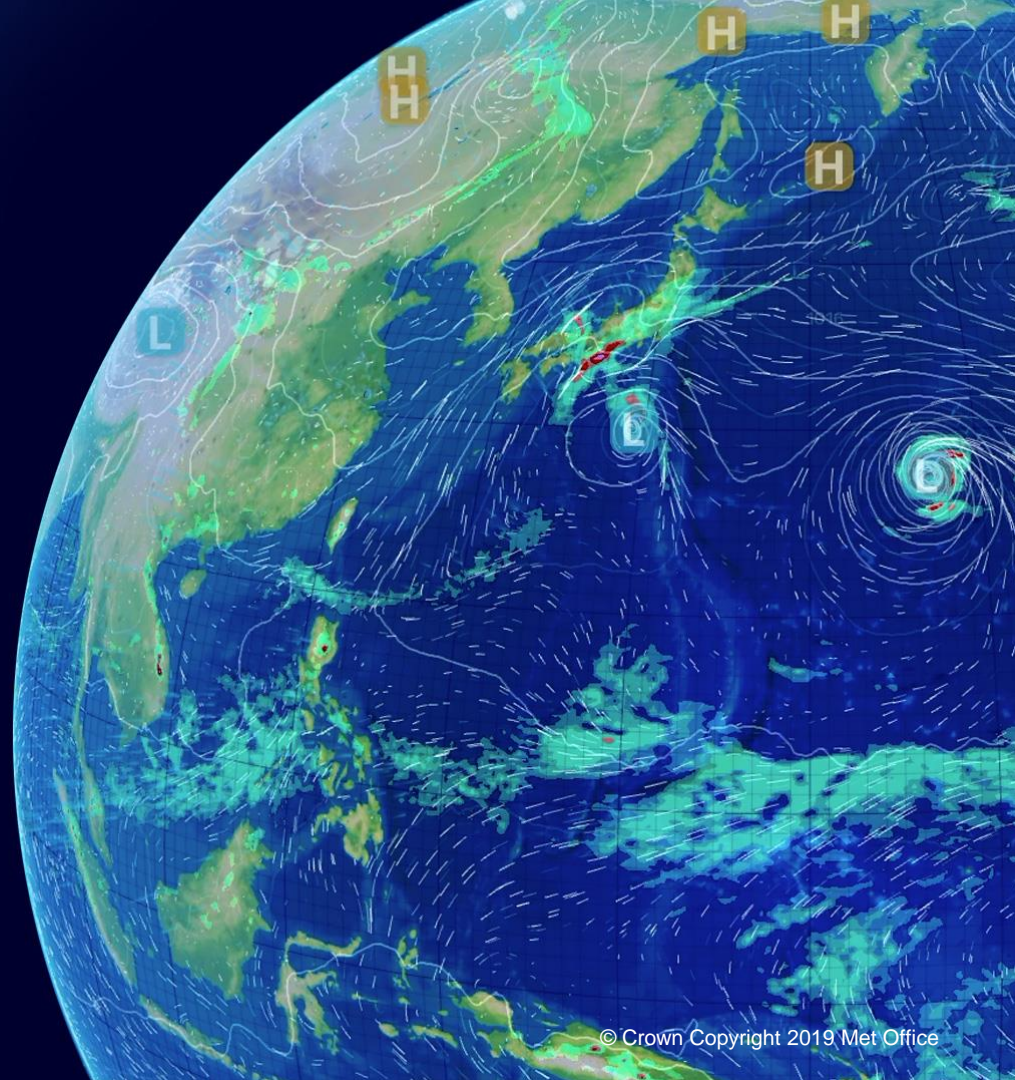# ExCALIBUR webinar

21 November 2019

Met Office

Agenda

- Welcome
- Strategic Priorities Fund and ExCALIBUR landscape
- EPSRC funding call information
- Met Office funding call information
- Met Office procurement process
- Q&A session

SPF / ExCALIBUR landscape

Becky McCoy

Met Office

Strategic Priorities Fund (SPF)

The Strategic Priorities Fund (SPF) is being led by UKRI to:

- drive an increase in high quality multi and interdisciplinary research and innovation;

- ensure that UKRI's investment links up effectively with government research and innovation priorities and opportunities; and

- ensure the system responds to strategic priorities and opportunities.

• SPF builds on Paul Nurse's vision of a 'common fund', to support high quality multidisciplinary and interdisciplinary research programmes, which could have otherwise been missed through traditional funding channels.
https://www.ukri.org/about-us/strategic-prospectus/how-we-will-deliver-and-measure-success/

Exascale Computing: ALgorithms and Infrastructures Benefiting UK Research - ExCALIBUR

Aim: To redesign high priority simulation codes and algorithms to fully harness the power of future supercomputers, keeping UK research and development at the forefront of high-performance simulation science.

Challenge: Radical changes to supercomputer architectures are on the horizon. To continue to make scientific advances on some of the most challenging physical problems, such as weather forecasting, engine design, astrophysics, particle physics and fusion energy, it is essential that the UK fully harnesses the power of those supercomputers.

Approach: Collaboratively work together to future proof the UK against the fast-moving changes in supercomputer designs. This combined scientific expertise will push the boundaries of science across a wide range of fields delivering transformational change at the cutting-edge of scientific supercomputing.

Delivery Partners: Led by the Met Office and EPSRC (on behalf of UKRI Research Councils) along with UKAEA, NERC, STFC and MRC.

ExCALIBUR

Met Office

ExCALIBUR is based around four pillars:

Separation of Concerns: Maths of problem separated from computer science of implementation.

Co-design: Holistic, collaborative design of entire system by mathematicians, domain scientists and computer scientists.

Data Science: Research new workflows to manage & analyse vast volumes of simulation data.

Investing in People: Interdisciplinary RSE career development driven by forward-looking scientific software design.

Delivery activities include: High Priority Use Cases, Cross-cutting Research, RSE Knowledge Integration, Exploring Emerging Disciplines and Development of Novel Test Beds.
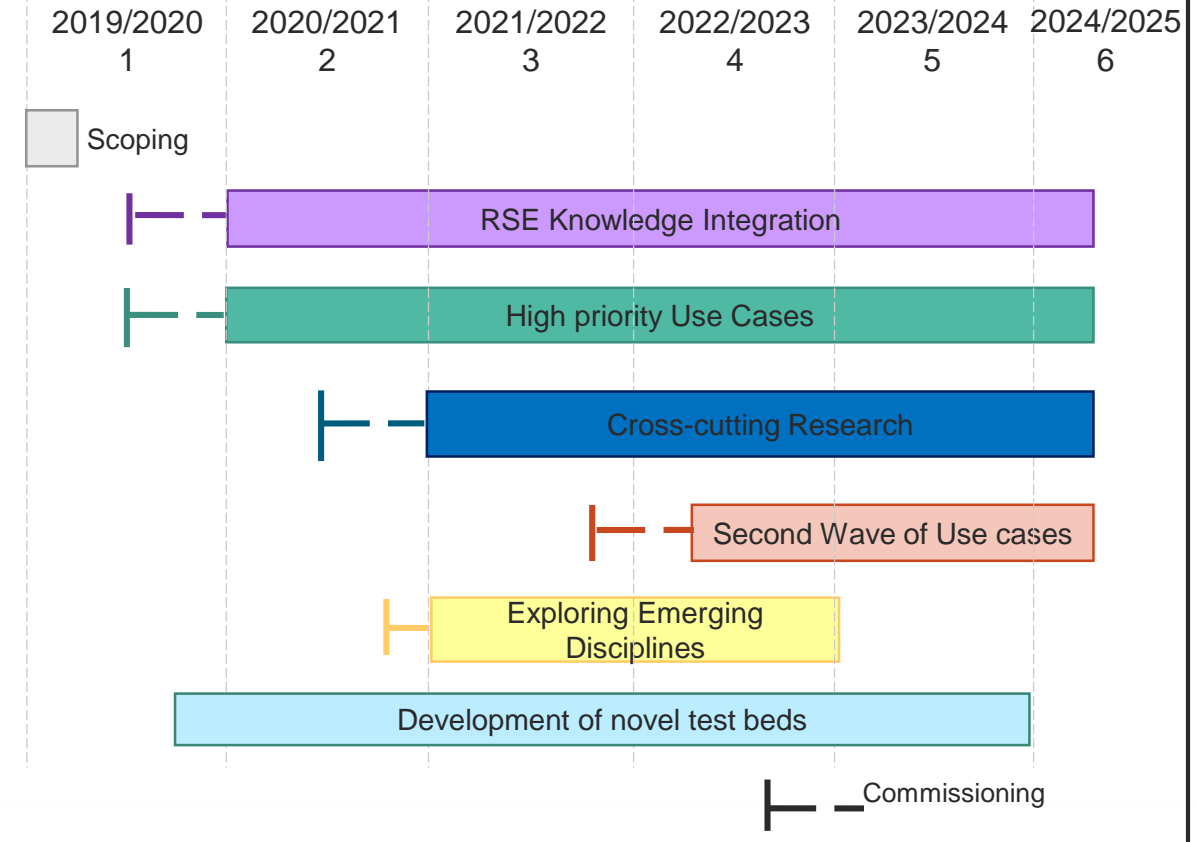
Figure 1. outlines the ExCALIBUR Programme in terms of the fundamental pillars of research and specific delivery activities.

UKRI UK Research and Innovation

Welcome

ExCALIBUR High Priority Use Cases: Phase 1 (Design & Development Working Groups)

Background

- **ExCALIBUR** (Exascale Computing Algorithms and Infrastructures Benefitting UK Research) is a £45.7m Strategic Priorities Fund (SPF) programme led by the Met Office and UK Research and Innovation to deliver research and innovative algorithmic development to harness the power of exascale HPC.

- ExCALIBUR will be delivered over five years through a suite of complementary activities delivered by UK Research and Innovation, the Met Office and UKAEA:

  - a **knowledge integration** activity;
  - activities to address **high priority use cases;**
  - supporting **emerging requirements for high-performance algorithms;**
  - **cross-cutting research**; and
  - **proof-of-concept hardware**.

- UK Research and Innovation expects to launch its first ExCALIBUR call, addressing the '**high priority use case**' theme, on 27 November 2019.

UK Research and Innovation

Approach

- The UK Research and Innovation contribution to the high priority use case theme will be delivered in three phases:

  - **Phase 1**: Design and Development Working Groups will bring together a wide range of domain experts, mathematicians, computational scientists, and Research Software Engineers (RSEs) to develop simulation codes for exascale computing that will have high impact and that can be applied by a wide range of users in strategically important areas of research.

  - **Phase 2**: Design and Development Working Groups will undergo independent expert review after 12 months. Successful Working Groups will be provided with the opportunity to secure further funding for research and development projects. At this stage, there will be opportunities for new entrants to apply to participate in research and development projects.

  - **Phase 3**: a second wave of use case calls will be launched at a later stage.

UK Research and Innovation

Scope

- A '**high priority use case**' has the following characteristics:

    - Enables high quality, high impact research in multiple areas of strategic importance;

    - Provides a step-change in simulation performance and/or provide solutions that are not currently feasible, consistent with the enhanced performance of exascale computing;

    - Applicable and scalable solutions that can be applied across a range of architectures, including non-exascale systems;

    - Provides a national and international focal point for the relevant research communities, including the development of partnerships with complementary initiatives in the UK and internationally.

- This call is complementary to a parallel programme of activities led by the Met Office and the UK Atomic Energy Authority to address high priority use cases in the areas of **weather and climate prediction**, and **fusion modelling**. Accordingly, proposals focussed on these areas will be out of the scope of this call.

UK Research and Innovation

Design and Development Working Groups

- Working Groups bring together a wide range of expertise (subject matter experts, RSEs, computational scientists, mathematicians etc.) to scope and progress simulation code design and development activities for exascale computing.

- Working Groups are expected to:

  - bring together a community of practice focussed on addressing a specific high priority use case;
  - conduct a mixture of exploratory research and development and community building activities;
  - collaborate with other working groups and potential beneficiaries;
  - develop a strategic research agenda and conduct proof-of-concept studies.

UK Research and Innovation

Next steps

- Up to £1.2m is available to support approximately 4-8 Working Groups (i.e. £150-300k per proposal).

- Working Groups will have a duration of 15 months from 1 April 2020.

- Applicants working in any field of research supported by UK Research and Innovation are invited to apply.

- A kick-off workshop will be organised by UK Research and Innovation at the start of the awards to facilitate collaborative working between Working Groups, the Met Office, UK Research and Innovation and UKAEA.

UK Research and Innovation
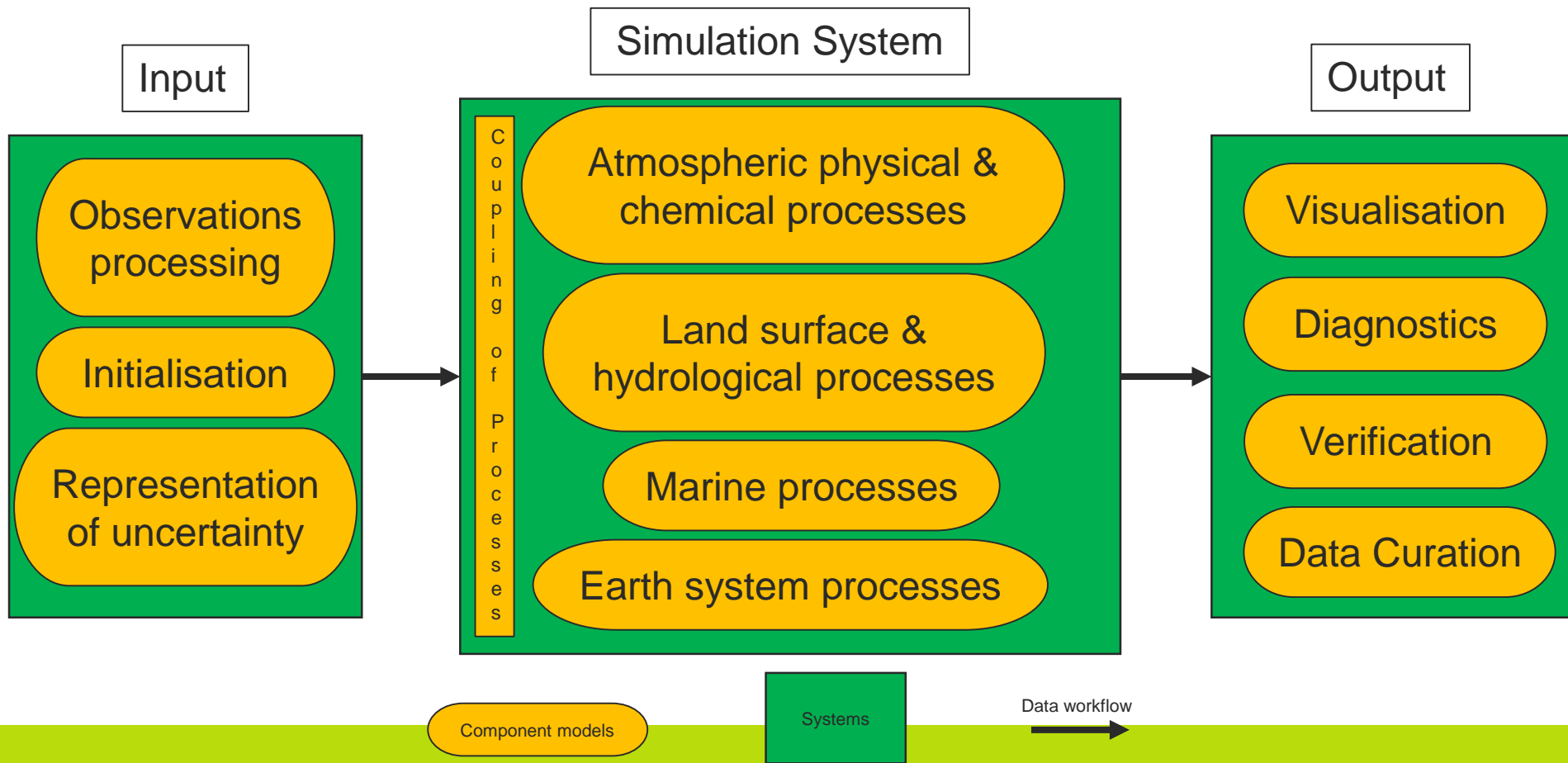
Call dates (TBC)

Activity	Date
Call opening date	27 November 2019
Call closing date	22 January 2020
Expert panel	w/c 24 February 2020
Funding decision	March 2020
Grant start date	01 April 2020
Grant end date	31 June 2021

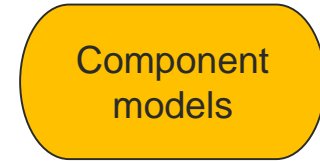UK Research
and Innovation

ExCALIBUR funding calls

Nigel Wood
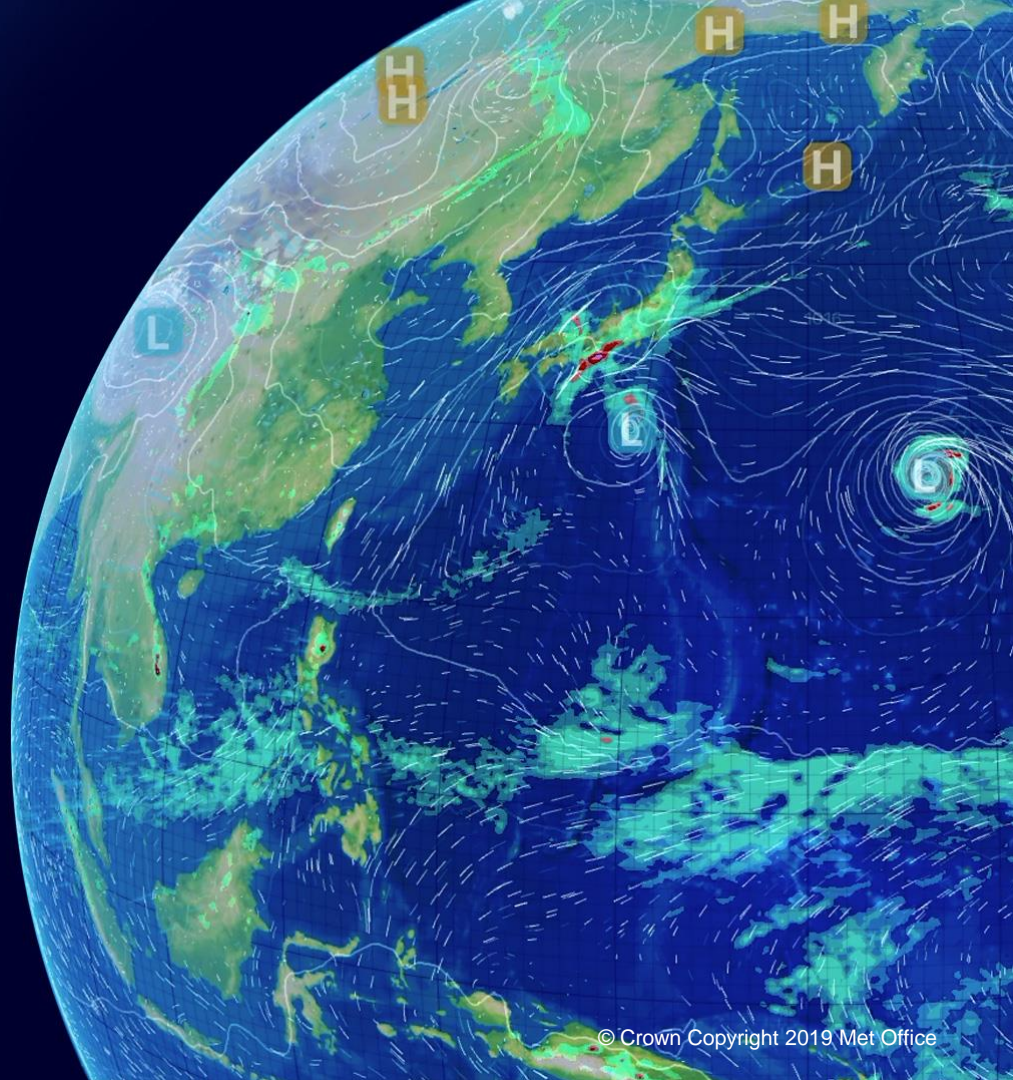
Met Office
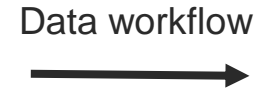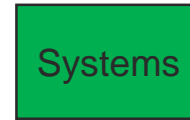
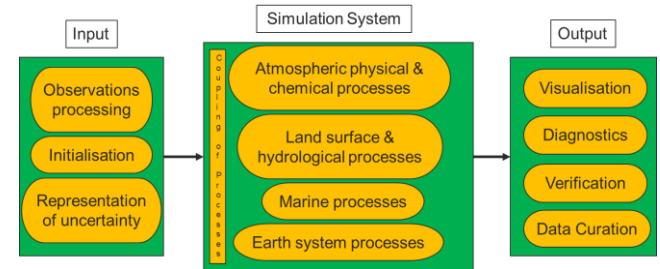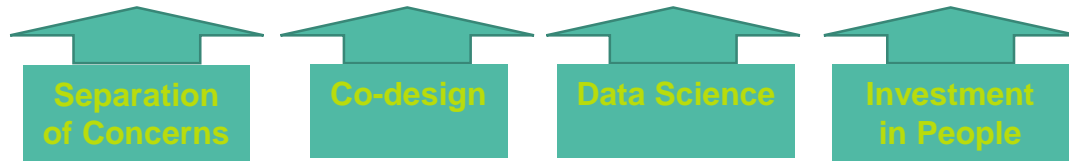Schematic of weather & climate use case

Use case work packages

1. **Component models**

2. **System co-design**

3. **System integration**

Work Package 1 Activity 1:
UK Chemistry and Aerosol (UKCA) model design

UKCA is responsible for predicting large numbers of atmospheric chemical and aerosol species and their impact on climate, weather, and air quality.

Essential component across all time scales

Yet one of the most expensive

This activity will:

> Atmospheric physical & chemical processes

- Improve its computational performance

- Improve its flexibility in terms of its ease of deployment to different architectures

- Improve its general usability

This will pave the way for coupling revised UKCA to the next generation system including use of a reduced resolution facility

Work Package 1 Activity 1:
UK Chemistry and Aerosol (UKCA) model design

This activity will:

Atmospheric physical & chemical processes

- Create a functioning stand-alone version of UKCA with its own driver, in an appropriate repository, and with its own testing strategy

- Deliver an analysis of the bottlenecks and hindrances to improved performance of UKCA on current and anticipated supercomputer architectures and recommend how to address those bottlenecks and hindrances

- Implement and test the most important modifications to deliver, with demonstration, a significant improvement in UKCA performance and flexibility

Work Package 1 Activity 2:
Marine Systems (NEMO) design

The weather & climate system has a number of marine systems, including:

Ocean (NEMO), Sea ice (SI^3), Ocean initialisation (NEMOVAR), and Biogeochemistry (MEDUSA)

Marine processes

These share same coding standards and specific code structure

Exploratory work with NEMO (the GOcean Technology Proof of Concept and more recent follow on work) has shown good potential to apply principle of separation of concerns without having to rewrite the source codes

This would extend the applicability of the current, CPU focused, codes to a much broader range of processor architectures, including GPUs.

Work Package 1 Activity 2:
## *Marine Systems (NEMO) design*

This activity will:

Marine processes

- Create an agreed strategy for a separation of concerns approach to the whole of NEMO in a way that means that the source code does not need to be directly modified

- Implement and demonstrate this strategy in an ocean-only context on CPUs and GPUs

- Apply the same approach to the other NEMO-like code bases in the priority order of: SI^3, NEMOVAR, MEDUSA

Bid submission process

Claire Gray
Met Office, Grants & Contracts Manager
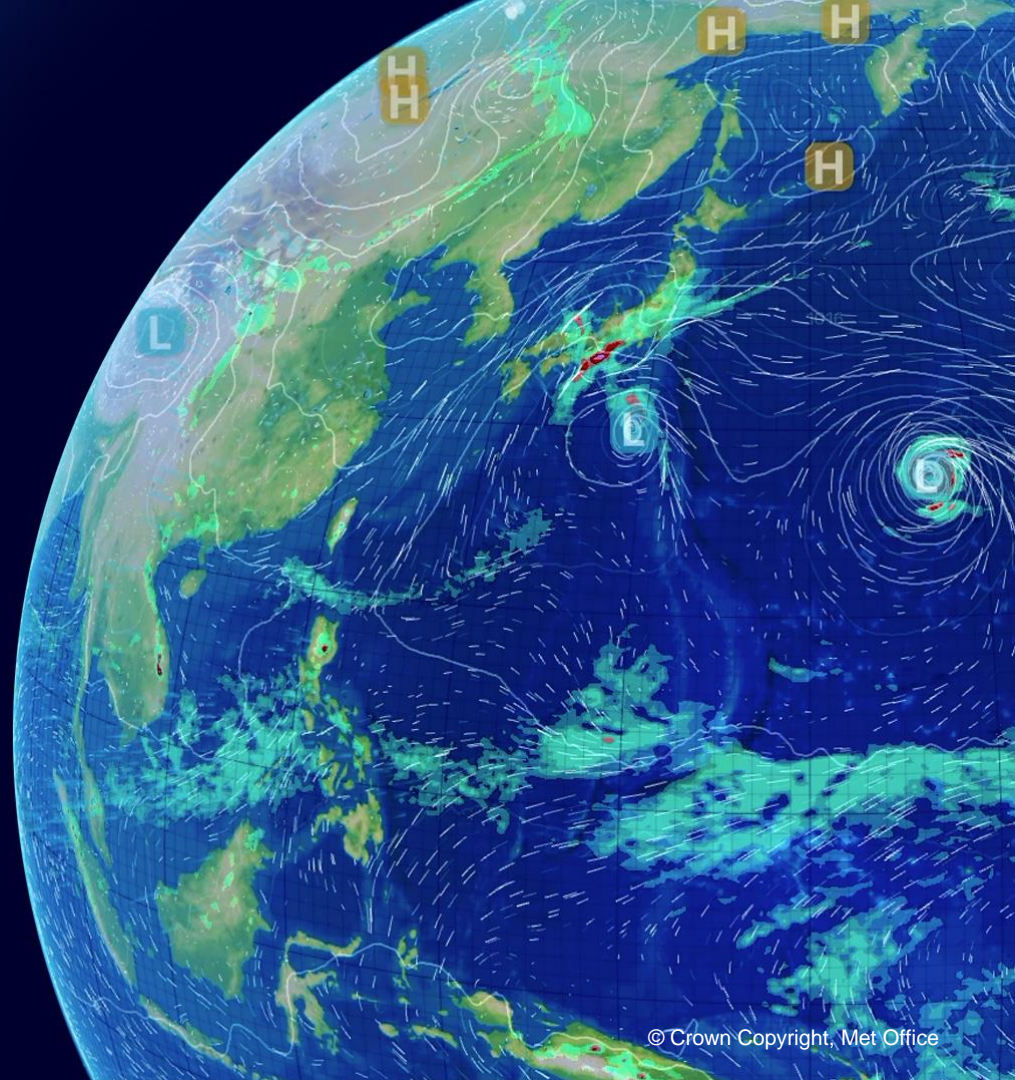
Procontract

- Procurement system for publishing and responding to EOI's and Calls
- Communication forum for all related Q&A

Met Office Procontract

- Suppliers can set up an account via this link- https://procontract.due-north.com/Login

Register free with ProContract

Begin your ProContract supplier account registration by filling in a few details below.

Organisation name

Email address

By clicking 'Continue registration', you agree to the Terms and Conditions & Privacy policy.

Continue registration

Already registered? Log in here

Why should I register with ProContact?
Registration is free and your company profile will be immediately available for opportunities managed by over 30,000 buyers from over 400 private, public sector and 3rd sector organisations.

What happens next?
Once we have verified your company name and email address you will be asked to complete a short registration process including basic company details and contact information. Upon submission, your registration application will be reviewed by the ProContract team and you will be sent an email address confirming next steps.

Do I receive opportunity alerts?
Following successful registration, as part of your company profile you can stipulate your preferred opportunity areas of interest along with geographical locations to which you can supply your goods & services. Overnight, your interests will be matched against the latest published opportunities and you will be notified by email. The email will contain links to review, and if you wish, express your interest in each of the opportunities.

- Further guidance will be given to potential bidders when each call is released through the Met Office website.

Call details

Work Package 1 Activity 1: UK Chemistry and Aerosol (UKCA) model design

- Up to value of £400k (100% FEC)
- 01/06/2020 – 31/03/2022

Work Package 1 Activity 2: Marine Systems (NEMO) design

- Up to value of £400k (100% FEC)
- 01/06/2020 – 31/03/2022

Call documents

Met Office

Document 1

Part 1: Background Information

Instructions

Background to grant and programme

Call / Lot specification

Evaluation and scoring process

Document 2

Part 2: Bidders to complete

- Eligibility
- Compliance Assessment
- Certification and Declaration
- Terms and Conditions

Document 3
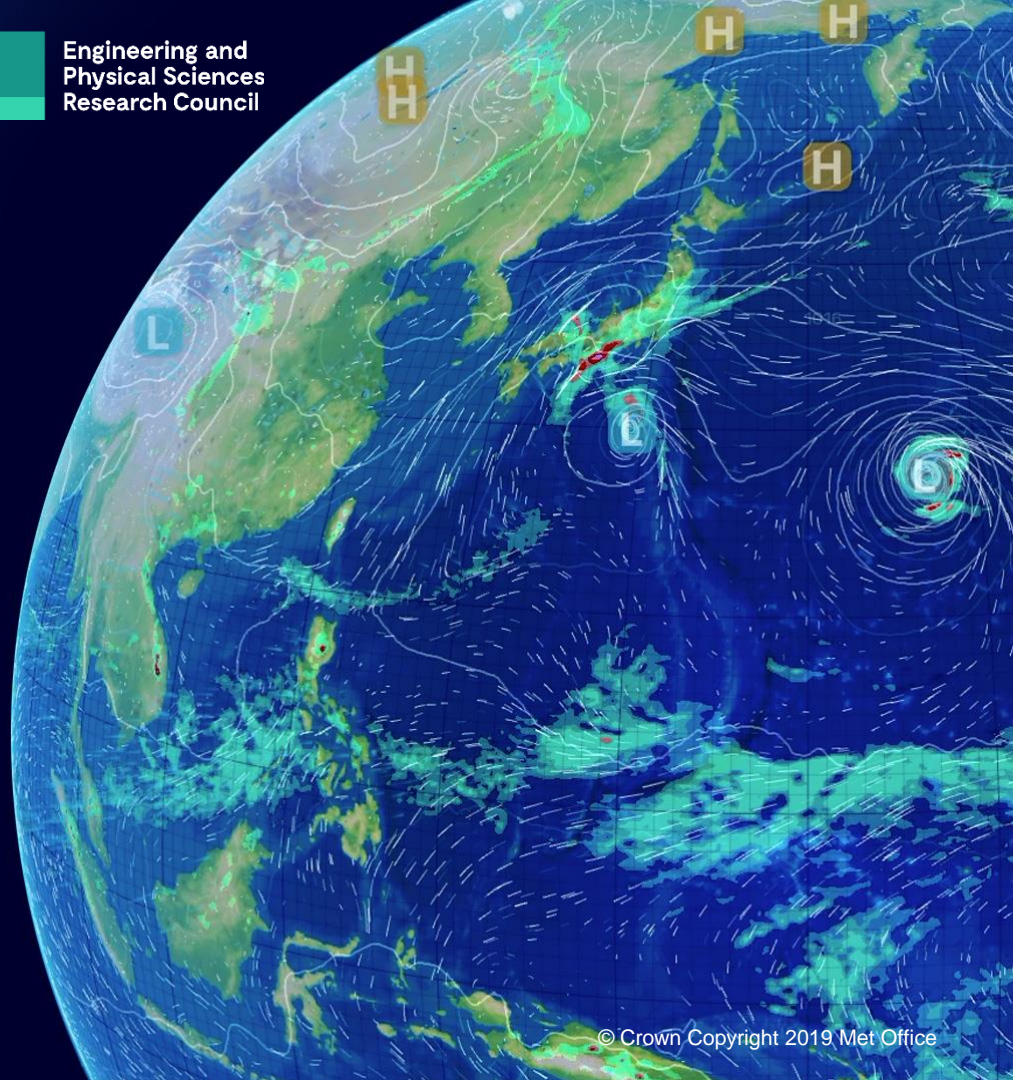
Research Plan: Bidders to complete

- Key Deliverables
- Activity Plan
- Resource Plan
- Risks
- Financial Breakdown

Indicative Timescales

EOI:	Early December 2019
Calls published:	Early January 2020
Bidding Period:	8 weeks (to close Mid-March 2020)
Award of Call:	April 2020
Delivery Period:	01/06/2020 – 31/03/2022

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