EXCALIBUR 10

HARNESSING EXASCALE COMPUTING – AN EXCALIBUR OVERVIEW

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Met Office

UKRI UK Research and Innovation

UK Atomic Energy Authority

Strategic Priority Fund (SPF)

The SPF builds on the vision of a ‘common fund’ set out in Sir Paul Nurse’s review.

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 priorities and opportunities
- and ensure the system responds to strategic priorities and opportunities.

Two waves of programmes

34 themes of research

Harnessing Exascale Computing

Exascale Computing ALgorithms & Infrastructures for the Benefit of UK Research (ExCALIBUR

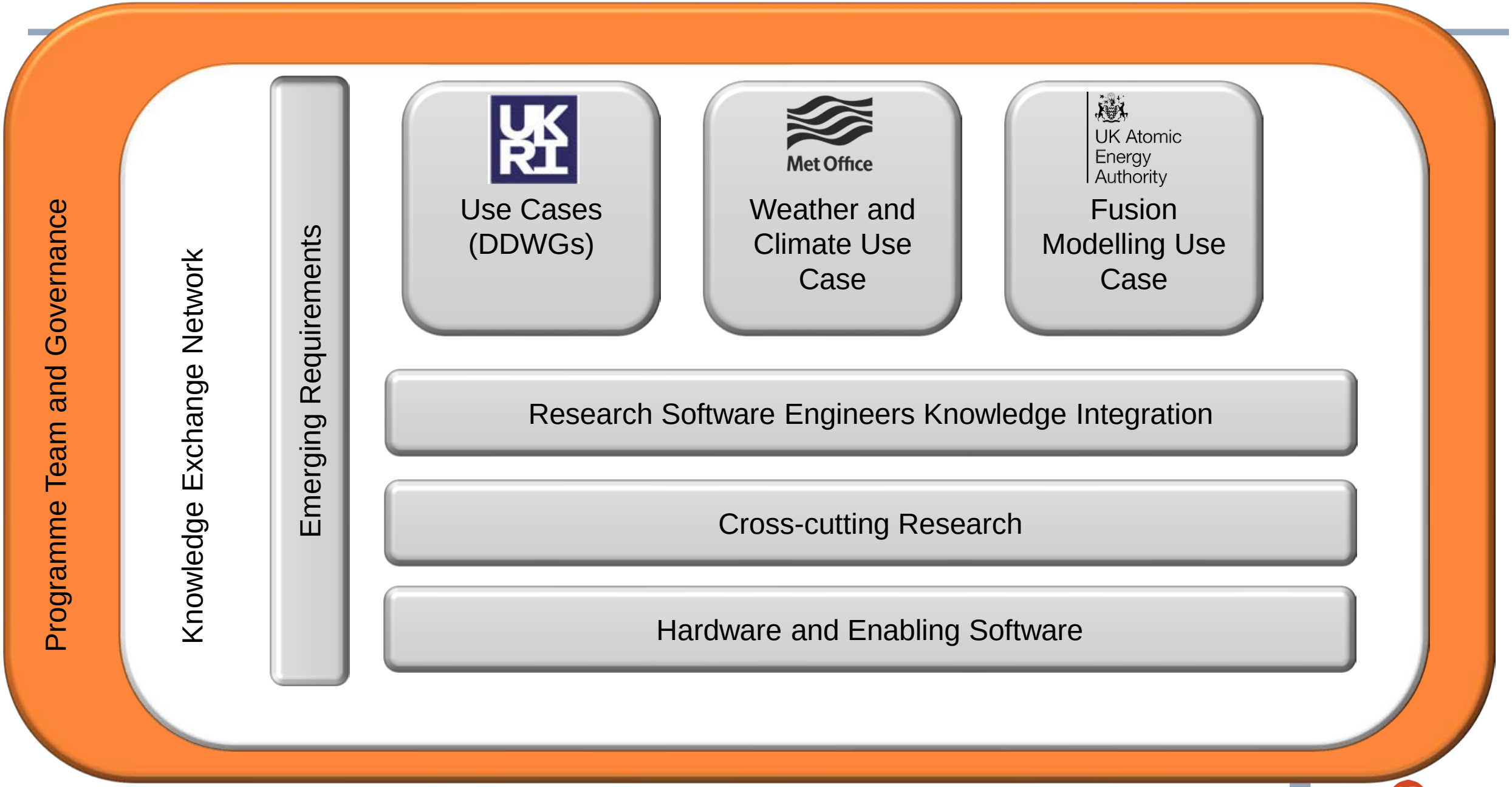
- Lead Delivery partners: Met Office (PSREs) + EPSRC (UKRI)
  - Delivery Partners: UKAEA, STFC, NERC, MRC
- ***Aiming to redesign high priority simulation codes and algorithms to fully harness the power of future supercomputers, keeping UK research and development at the forefront of high-performance simulation science***

Separation of Concerns: Each concern is addressed by distinct parts of the software. Maths of problem separated from computer science of implementation.

Co-design: Holistic design of entire system. Innovative collaborations between mathematicians, domain scientists and computer scientists.

Data Science: Research to design new workflows adapted to managing & analysing vast volumes of data ingested and produced by simulations.

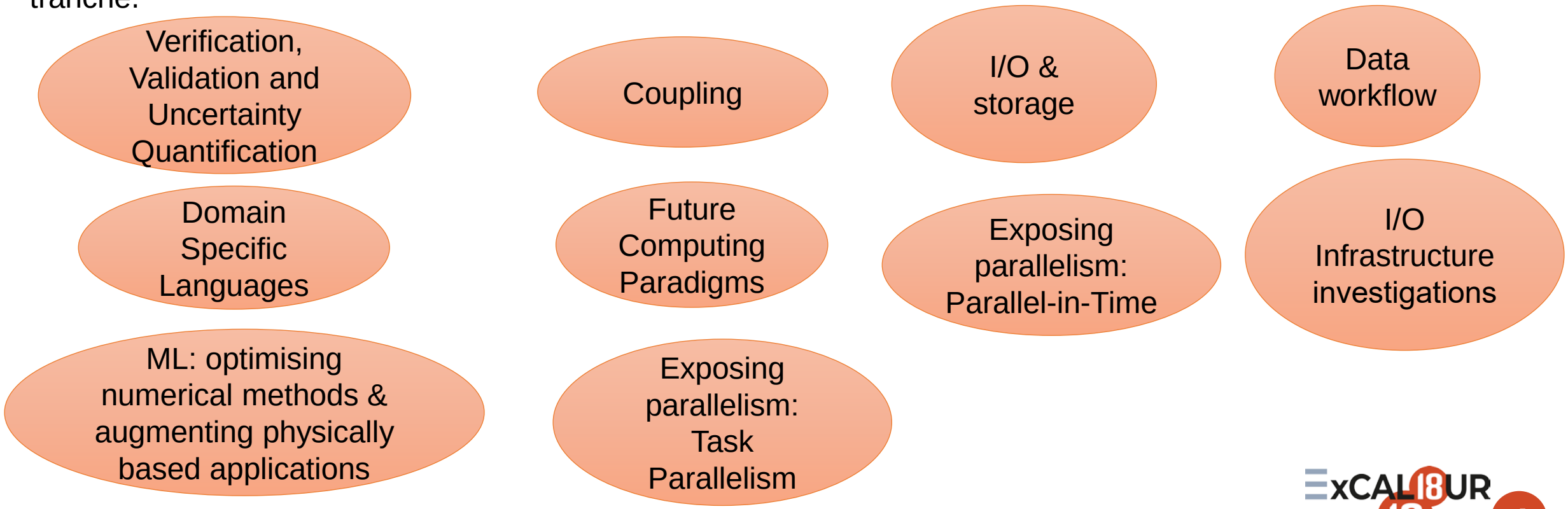
Investment in People: Improved RSE career development driven by professional forward-looking approach to scientific software design of simulation codes.



What is Cross-cutting Research?

- Co-ordinated approach addressing known technology/infrastructure issue if resolved will lead to significant progress across range of exascale software development challenges

- We invited the wider community to help scope the themes of research that should be addressed in this tranche.



Cross-cutting Research Awards

Principal Investigators

Containers
- Dr Stuart Whitehouse, Met Office

Coupling
- Professor Garth Wells, University of Cambridge

Data workflow
- Professor Bryan Lawrence, University of Reading

Domain Specific Languages
- Dr Tobias Grosser, University of Edinburgh

Exposing parallelism: Parallel-in-Time
- Dr Jemma Shipton, University of Exeter and Imperial College London

Exposing parallelism: Task Parallelism
- Professor Tobias Weinzierl, Durham University and STFC Hartree

Future Computing Paradigms
- Dr Vivien Kendon, Durham University

Future Computing Paradigms
- Professor Jason McEwen, University College London

Verification, Validation and Uncertainty Quantification
- Professor Peter Challoner, University of Exeter

Verification, Validation and Uncertainty Quantification
- Professor Peter Coveney, University College London

I/O & storage
- Professor Bryan Lawrence, University of Reading, NCAS and University of Cambridge

I/O Infrastructure investigations
- Dr Stuart Whitehouse, Met Office

Machine learning: optimising numerical methods and augmenting physically based applications
- Dr Amy Krause, University of Edinburgh, EPCC

Workflow Design and Analysis
- Dr Stuart Whitehouse, Met Office

Knowledge Exchange

Identify and lead on opportunities for Knowledge Exchange at project level

Increase the awareness of your project and the ExCALIBUR programme

Collaborate with relevant academic, industrial and international communities

Collaborate as a network with other ExCALIBUR Knowledge Exchange co-ordinators to deliver activities and facilitate knowledge sharing

Knowledge Exchange Co-ordinators

Containers, I/O Infrastructure investigations, Workflow Design and Analysis
- Dr Stuart Whitehouse, Met Office

Coupling
- Dr Chris Richardson, University of Cambridge

Data workflow
- Dr Fanny Adloff, University of Reading

Domain Specific Languages
- Dr Nick Brown, University of Edinburgh

Exposing parallelism: Parallel-in-Time
- Dr Jemma Shipton and Professor Beth Wingate, University of Exeter

Exposing parallelism: Task Parallelism
- Dr Marion Weinzierl, Durham University

Future Computing Paradigms
- Dr John Buckeridge, London South Bank University

Future Computing Paradigms
- Dr Harpreet Dhanoa and Dr Jeremy Yates, University College London

Verification, Validation and Uncertainty Quantification
- Dr Derek Groen, Brunel University

Verification, Validation and Uncertainty Quantification
- Dr James Salter, University of Exeter

I/O & storage
- Dr Fanny Adloff, University of Reading, NCAS

Machine learning: optimising numerical methods and augmenting physically based applications
- Dr Amy Krause, University of Edinburgh, EPCC

UKRI Use Cases

A phased approach

Design and Development Working Groups

- ELEMENT - Exascale Mesh Network
- Materials And Molecular Modelling Exascale Design And Development Working Group
- Gen X: ExCALIBUR working group on Exascale continuum mechanics through code generation
- Exascale Computing for System-Level Engineering: Design, Optimisation and Resilience.
- Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics
- Benchmarking for AI for Science at Exascale (BASE).
- Lattice Field Theory at the Exascale Frontier
- ExaClaw: Clawpack-enabled ExaHyPE for heterogeneous hardware
- ExCALIBUR-HEP (= High Energy Physics)
- Turbulent Flow Simulations at the Exascale: Application to Wind Energy and Green Aviation

A co-ordinated range of activities, which aims to develop simulation code with a focus on an application or applications pre-identified by the relevant communities as benefitting from exascale software development.

Announcement of awarded projects will take place in the new year.

RSE Knowledge Integration

Developing expertise

- Create an evolving training curriculum encompassing both technical and professional development.
- Work towards growth in number of the UK RSE Community across both academia and industry.
- Focus on the development of activities to facilitate both the cross fertilisation of knowledge and the movement of people within and between academia and industry.

Phase 1: Landscape Review

Phase 2: Funding Opportunity

Training and skills embedded in call requirements

Landscape Review

- The skills required by RSEs in HPC.
- The future training needs of RSEs.
- Challenges faced in developing these skills and growing the number of RSEs in the UK with a specific focus on HPC.
- The importance of establishing a career path for RSEs that does not rely on the conventional academic metrics.

Hardware and Enabling Software Group

- H&ES is an initiative set up to trial prototypes and testbeds of a number of potential next generation supercomputing systems and supporting software such as compilers for the use of ExCALIBUR projects and the wider UKRI community.

- Jointly led by Rev Dr Jeremy Yates and Professor Simon McIntosh-Smith. Programme Co-ordinator Martin Hamilton

    - Delivers annual calls to support novel hardware/software testbeds for prototyping and development

    - Lead benchmarking activities
        - Surveying ExCALIBUR projects to understand their exascale benchmarking requirements
        - Working with ExCALIBUR projects to collate and package exascale benchmarks ready for novel architecture

Highlights and Updates

Highlights

- Delivery of numerous workshops, training and scoping activities held by DDWGs since 2019 to develop their use cases
  - Code performance series, Podcast series, Firedrake training, Deep Dive talks
- Series of Cross-cutting workshops and kick off meetings held
  - Task Parallelism: Performance Analysis Methodology workshop
- H&ES have secured general access for ExCALIBUR projects to the first wafer scale accelerator system in Europe (EPCC with Cerebras and HPE)
- First cluster based on NVIDIA Arm Developer Kit in the EMEA region (Leicester with NVIDIA and Arm)

Upcoming opportunities

- Emerging Requirements – to prepare communities and understand their software requirements
- UKRI Use Cases Phase 2 – ensure a balance across the portfolio of UKRI Use Cases supported

Contact us

Visit our website:
www.excalibur.ac.uk

Sign up to Knowledge Exchange Annoucements mailing list:
https://jiscmail.ac.uk/excalibur-ke-annouce

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