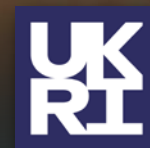# ExCALI8UR 10

PROGRAMME OVERVIEW

Presenter

Billy McGregor

UKCTRF Presentation, April 2021

Met Office

UKRI — UK Research and Innovation

UK Atomic Energy Authority

Background to the ExCALIBUR programme
Current UK Landscape

- What is supercomputing and what is exascale software?

- Why does it matter for the UK?

- What is the timeline for exascale software in the UK/Europe/USA/Worldwide?

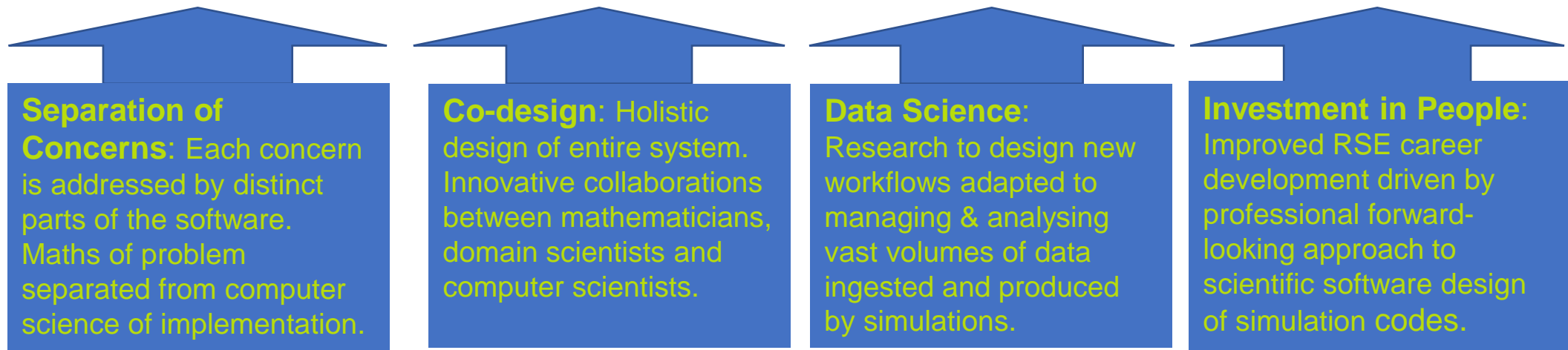- UK Research & Innovation: Science case for UK Supercomputing

Strategic Priority Fund

- 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
  - 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/.)

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Harnessing Exascale Computing

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

- 5 year programme

- Delivery partners: Met Office (PSREs) + EPSRC (UKRI)

- *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.

UKRI SPF Wave 2: Met Office, UKAEA, EPSRC, STFC, NERC, MRC

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Programme Delivery

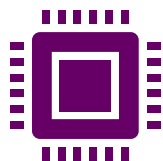RSE Knowledge Integration (~£750k, yrs 1-5)

High Priority Use Cases (~£26m, yrs 1-5)

Emerging Requirements for High Performance Algorithms (~£3m, yrs 2-3)

Cross-cutting Research (~£10m, yrs 2-5)

Hardware and Enabling Software (~£4.5m yrs 1-5)

Progress of ExCALIBUR to date
Headlines

- Timeline of the ExCALIBUR programme

- Funded UKRI and Met Office projects

- Current and future calls

- Website

Use Cases

UKRI – 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

Cross-cutting approach

- Co-ordinated approach addressing known technology/infrastructure issue
- Resolution will lead to significant progress across range of exascale software development challenges
- Apply to multiple Use Cases
- Utilise the lessons learnt from the use cases and design and development working groups to address common issues that impact scientific code under development for use at exascale
- Needs to include contributors from beyond the Use Cases – should be domain agnostic (within remit of ExCALIBUR)
- ExCALIBUR two cross-cutting work packages:
  1. **Common approaches and solutions**
  2. **Potential disruptors**

Future Opportunities

Calls over the remainder of the programme

- Cross cutting call (UKRI) - Open

- Use case phase 2 - Opens early 2022

- RSE phase 2 – Opens 2021/2022

- Emerging Requirements Call – Opens 2022

- Met Office opportunities

- UKAEA opportunities

Thank you!

Web: **Met Office ExCALIBUR web pages**

Email: **SPF Programme Office**

Twitter: **@metoffice_sci, @ukri_news, @epsrc**

LinkedIn: **UK Research and Innovation**

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