Exalat kick-off workshop

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What is Exalat?

- Working Group funded as part of ExCALIBUR - UKRI (apologies for the occasional UK jargon)

- *It should enable effective engagement between the computational research community and **research communities** that can benefit from exascale computing. Their aim should be 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**. The outputs of these Working Groups will contribute to future elements of the ExCALIBUR programme.*

ExCALIBUR

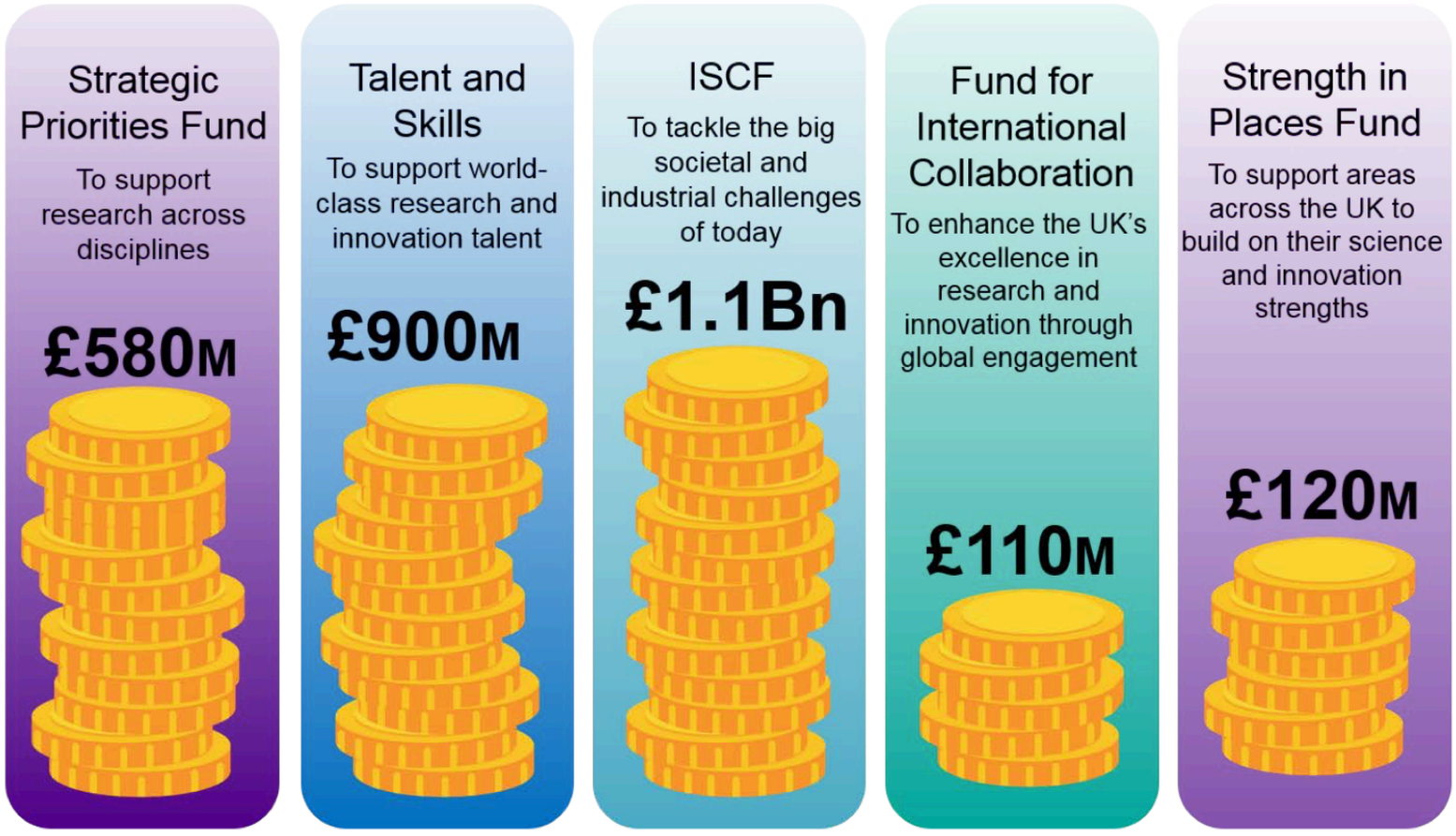
Exascale Computing: ALgorithms and Infrastructures Benefiting UK Research

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.

Plan for Exalat

- Wide scientific portfolio of the LFT community
- Identify:
    - current state-of-the-art
    - opportunities, readiness/benchmarks, requirements, hardware
    - training, human resources
- Links with other communities
- What happens elsewhere?

National Productivity Investment Fund



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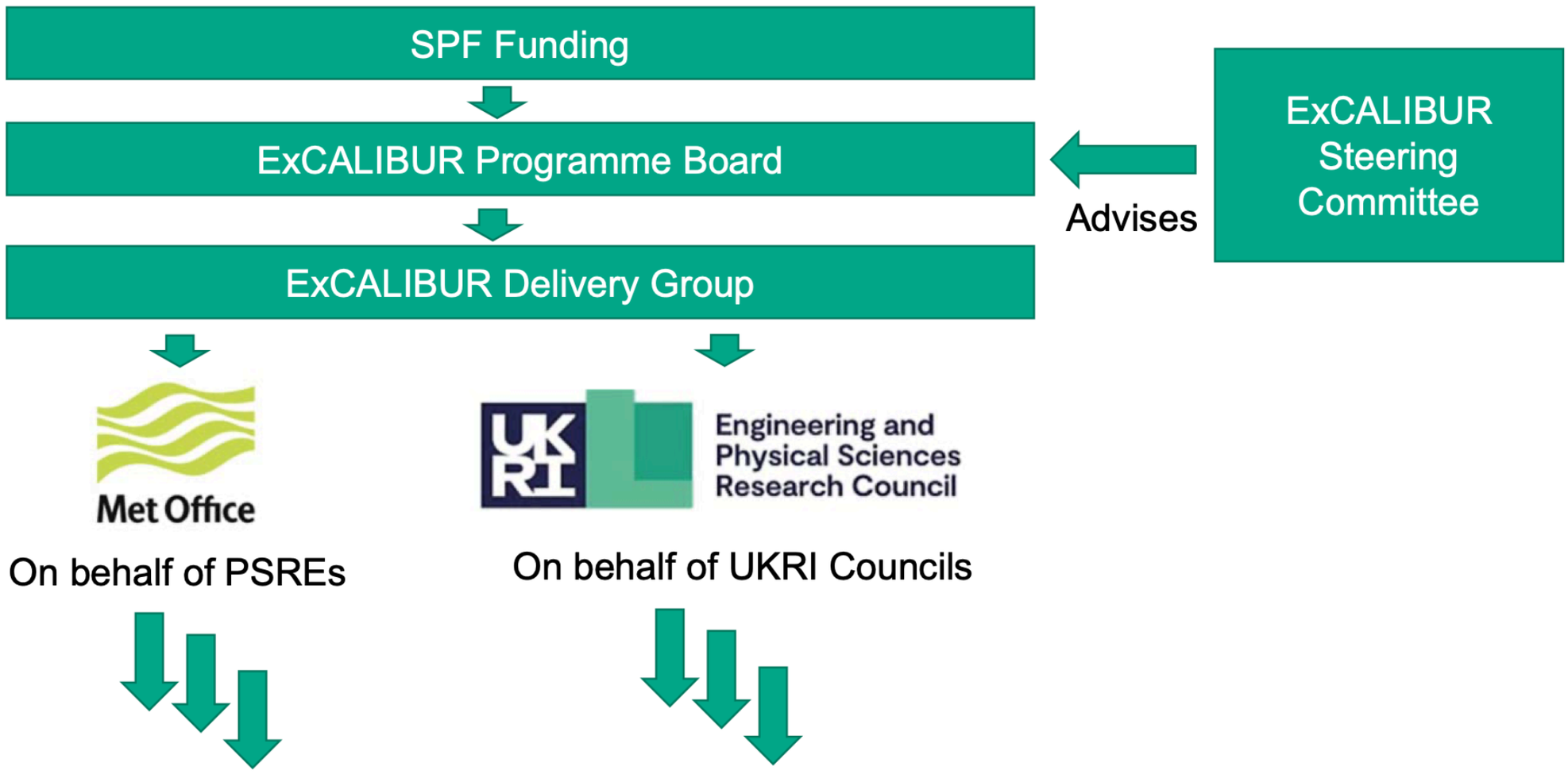
Programme structure



The ExCALIBUR approach

Efficiency | ***Capability*** | ***Expertise***

Separation of Concerns: the maths of problem is separated from the computer science of implementation

Co-design: holistic, collaborative system design by mathematicians, domain scientists and computer scientists

Data Science: new workflows to manage and analyse vast volumes of simulation data

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

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Algorithmic Approach – Derived from activities

- The Exascale definitions we will use are activity based:
  - Solving Problems that are a 10-1000x larger than we solve at present
  - Solving Problems 10-1000 faster than at present
  - Problems can be simulation, data modelling and/or data driven
  - Can come from all areas of Research and Innovation
  - Exascale “Velocity” is just an important output as Exascale “Volume”
- These are the drivers of algorithmic design

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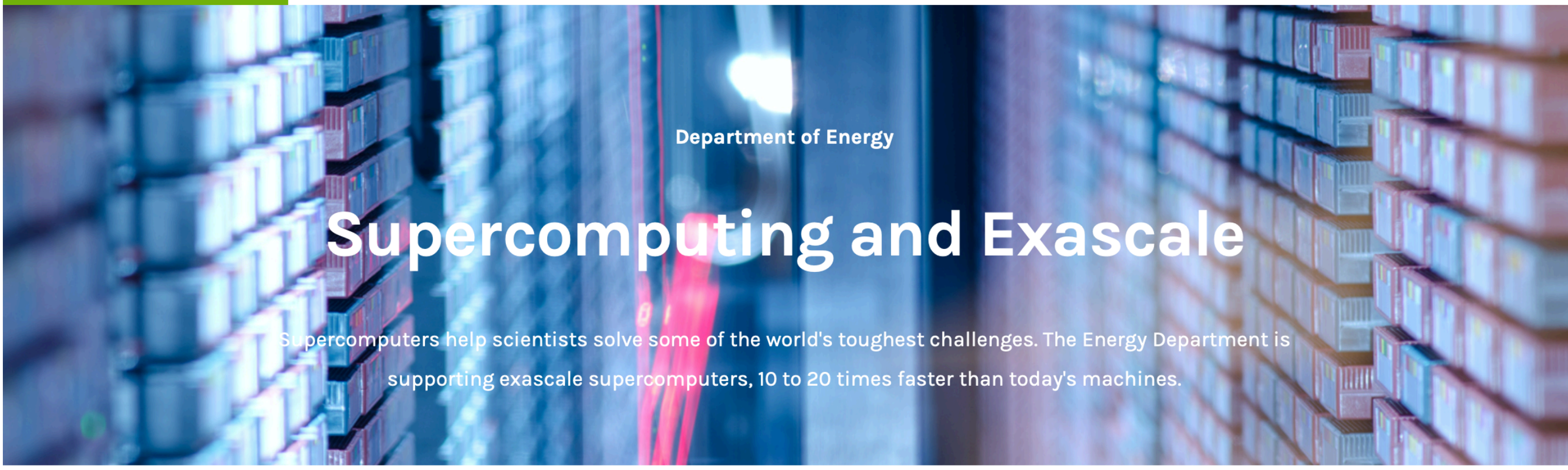

Several machines in the US - heterogeneous architectures

- Summit
- Frontier
- Aurora
- El Capitan

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EuroHPC

Leading the way in the European Supercomputing

The EuroHPC Joint Undertaking is a 1 billion Euro joint initiative between the EU and European countries to develop a World Class Supercomputing Ecosystem in Europe.

Pre-exascale systems being deployed

Possible funding for exascale systems in the next MFF

158,976 A64FX processors - yet another architecture

Building a roadmap

Physics/Hardware and Software:

- What are the physics objectives that would be possible/desirable with Exascale machines?
- What are the required processing resources that are needed to execute these simulations?
- Which codebases and algorithms are or will be used, including their performance and scaling?
- Which HPC facilities and what hardware is or will be used?
- What are the potential bottlenecks on future hardware (x86, GPU, network, energy consumption, …)?

Maintaining leadership:

- How does the UK compare to other countries' roadmaps?
- What is the technology evolution of processing resources?
- How will stakeholders be able to design and write physics algorithms for these processing resources?
- How can coding standards and performance standards be used?
- What training opportunities do exist and what training will be required?
- Which are the connections with other domains, e.g. connections with ML (accelerating calculations, more efficient phase space sampling, lattice QCD, …)