Exalat kick-off workshop

Luigi Del Debbio

Higgs Centre for Theoretical Physics - The University of Edinburgh

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.
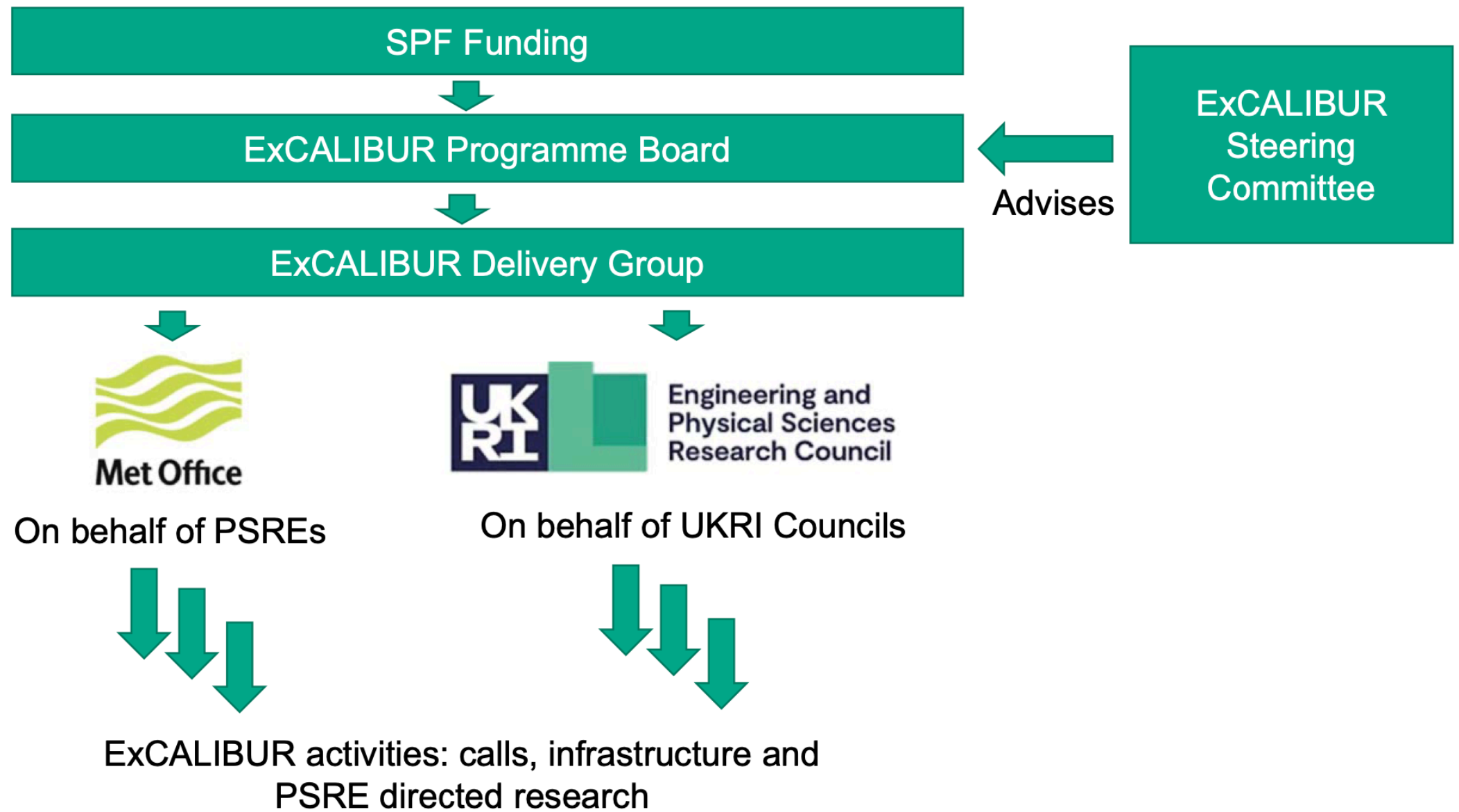
Plan for Exalat

- Interface with ExCALIBUR/UKRI: wide 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

Strategic Priorities Fund
To support research across disciplines
£580M

Talent and Skills
To support world-class research and innovation talent
£900M

ISCF
To tackle the big societal and industrial challenges of today
£1.1Bn

Fund for International Collaboration
To enhance the UK's excellence in research and innovation through global engagement
£110M

Strength in Places Fund
To support areas across the UK to build on their science and innovation strengths
£120M

UK Research and Innovation

Programme structure

SPF Funding

ExCALIBUR Programme Board

ExCALIBUR Delivery Group

ExCALIBUR Steering Committee

Advises

Met Office

On behalf of PSREs

UK RI — Engineering and Physical Sciences Research Council

On behalf of UKRI Councils

ExCALIBUR activities: calls, infrastructure and PSRE directed research

UK RI — UK Research and Innovation

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

UK Research
and Innovation

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

UK Research and Innovation

Department of Energy

Supercomputing and Exascale

Supercomputers help scientists solve some of the world's toughest challenges. The Energy Department is supporting exascale supercomputers, 10 to 20 times faster than today's machines.

Several machines in the US - heterogeneous architectures

- Summit
- Frontier
- Aurora
- El Capitan

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

9

RIKEN Post-K Supercomputer Named After Japan's Tallest Peak

By Tiffany Trader

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, …)

These are strange times…

thank you to all of you for being here, to the speakers, and to the LOC:

- Edinburgh/EPCC
- Plymouth
- STFC/Hartree — technical support in running the webinar
- Southampton
- Swansea