



UK Research  
and Innovation

# ExCALIBUR: an introduction

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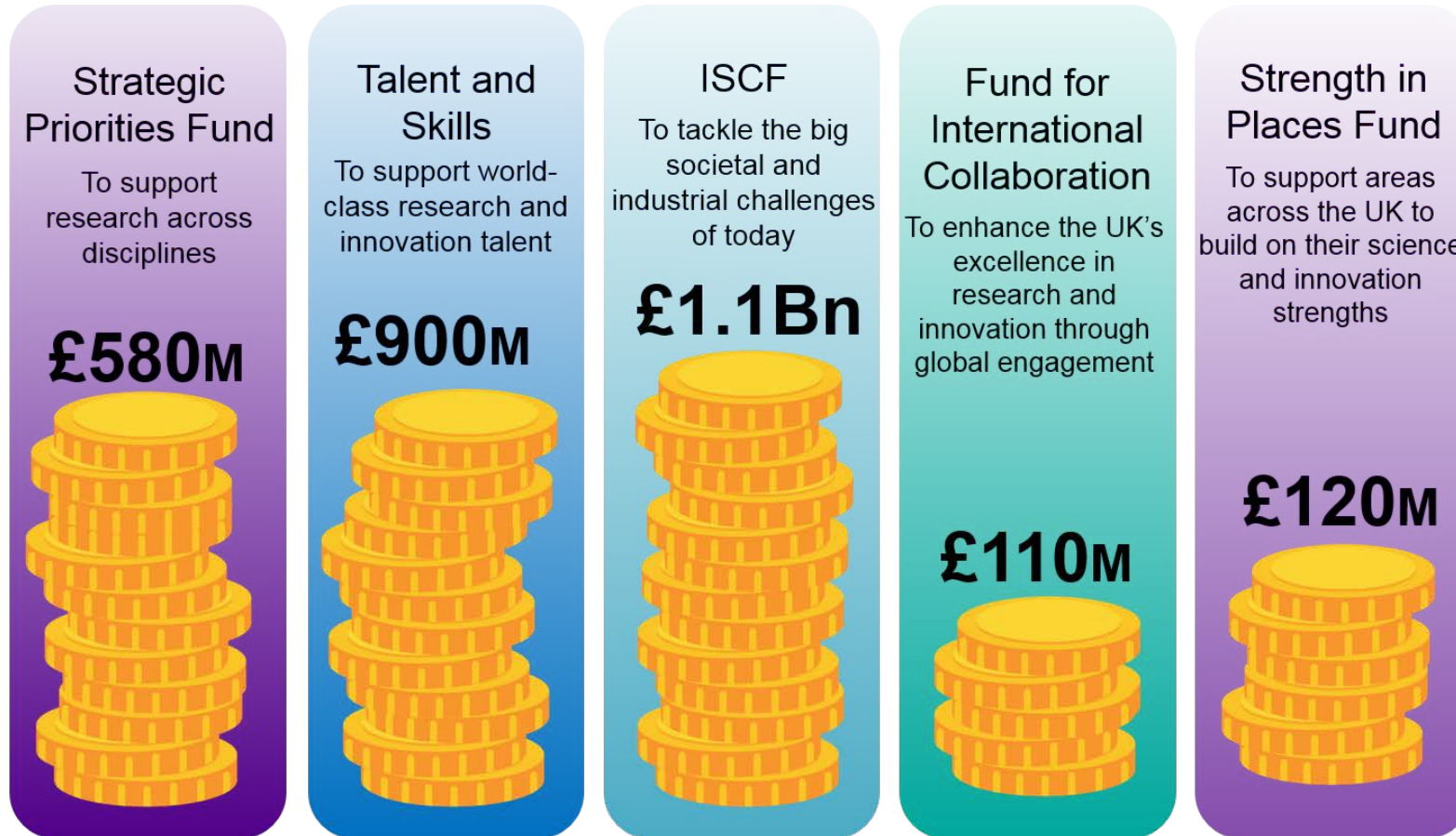


# Overview

1. Explaining the context, vision and importance of the Strategic Priorities Fund (SPF) and the ExCALIBUR programme.
2. Explaining the structure of the programme and planned activities.
3. Sharing and discussing opportunities for the RSE community to get involved.



# National Productivity Investment Fund



# Strategic Priorities Fund (SPF)

Established in 2018 and led by UKRI, the Strategic Priorities Fund (SPF) aims to:

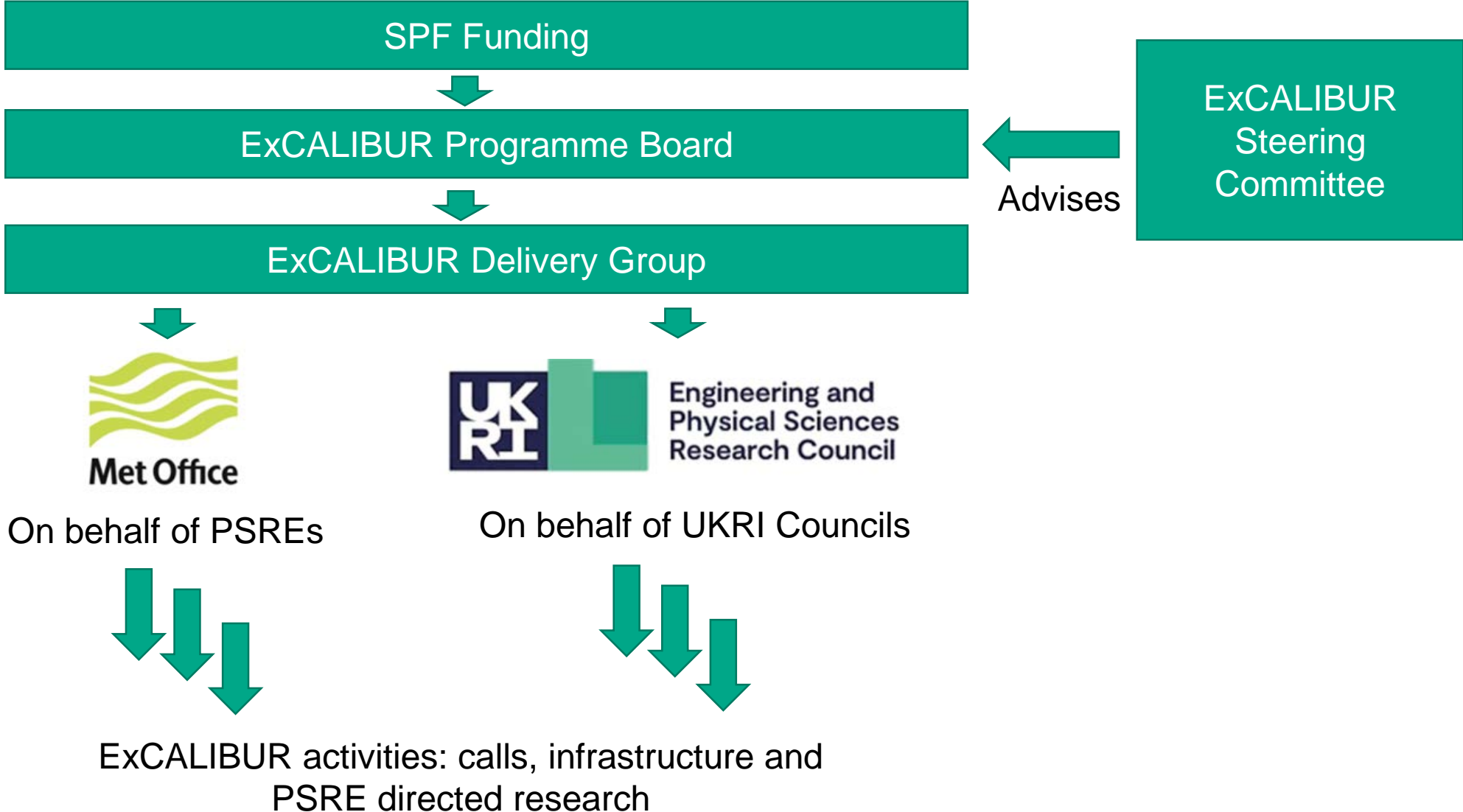
- drive an increase in **high quality multi and interdisciplinary** research and innovation;
- ensure that UKRI's investment **links up effectively with government** research and innovation priorities and opportunities; and
- ensure that the system **responds to strategic priorities and opportunities.**

SPF builds on Sir 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.

# Strategic Priorities Fund (SPF)

- The SPF portfolio consists of 34 programmes with a combined total investment of around £830m, funded in two ‘waves’.
- ExCALIBUR (Exascale Computing Algorithms and Infrastructures Benefitting UK Research) was awarded £45.7m of SPF funding in 2019.
- ExCALIBUR is a partnership between the UKRI Councils and Public Sector Research Establishments (PSREs) – led by EPSRC and the Met Office respectively – to harness the power of exascale HPC.

# Programme structure



# The ExCALIBUR approach

## *Efficiency*

**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



# The ExCALIBUR approach

<b>Efficiency</b>	<p>International academic research sees benefits through increased efficiencies in supercomputing enabling increased scientific output.</p> <p>Public and Government services that rely on high-performance simulations, e.g. weather forecasts, benefit from continued and improved services.</p>
<b>Capability</b>	<p>Academia and Industry using high-performance simulation codes see benefit through the implementation of the framework across disciplines which bring a step-change in capability.</p> <p>The Government sees benefit through the positioning of the UK as world-leaders in implementation and use of exascale supercomputing.</p> <p>UK plc sees benefits through transformational changes in capability in fields such as fusion modelling.</p>
<b>Expertise</b>	<p>Academic research and Industry will benefit from an interdisciplinary, agile RSE work force and an increase in two-way flow within and between academic and industry.</p> <p>UK plc will see benefit from an increase in productivity related to an increase in skilled RSE workforce.</p>



# Programme delivery



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



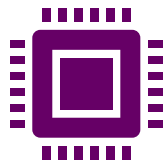
High Priority Use Cases (~£26m, yrs 1-5)



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)



# RSE Knowledge Integration



- Grow and Develop a multidisciplinary cohort of research software engineers (RSE's) who in collaboration with researchers will take on the fast-moving challenges in evolving supercomputer design.
- Build an evolving training curriculum to support the development of existing and new RSE's to meet the skills-gap arising from the changing demands of industry and academia.
- Provide a net outflow of highly-skilled workers into the UK economy
- RSE career development – create a new, forward-facing, interdisciplinary approach.

# High Priority Use Cases



- UKRI defines a ‘high priority use case’ as having the following features:
  - Enabling high quality, high impact research in multiple areas of strategic importance;
  - Providing 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;
  - Providing a national and international focal point for the relevant research communities, including the development of partnerships with complementary initiatives in the UK and internationally.

# High Priority Use Cases



- UKRI Use Case activities span the breadth of UKRI's remit.
- Met Office and UKAEA Use Cases are directed to weather & climate prediction and fusion modelling respectively.
- Initial UKRI ('Design and Development Working Groups', ~£2.5m) and Met Office activities launched in April 2020.
- Phases 2 (~£7.5m, Jul 21 – Apr 25) and 3 (~£4m, Apr 22 – Apr 25) of the UKRI Working Groups activity will provide further funding opportunities.
- A range of community engagement activities will take place over the coming months.



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# Questions?







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Welcome





# ExCALIBUR - an algorithmic approach to exascale design

Dr. Jeremy Yates, Joint-Lead ExCALIBUR Hardware and  
Enabling Software Programme

Prof Simon McIntosh-Smith, Joint-Lead ExCALIBUR  
Hardware and Enabling Software Programme

Dr. Rob Akers, Head of Scientific Computing, CCFE, UKAEA



# Structure of Talk – A framework

- What is an Algorithmic Approach to Computer Design
  - Creating a RSE-ResOps Alliance
  - Role of Hardware and Enabling Software Programme
- Separation of Concerns in Practice
- A list of Projects
  - Deep Dive into 2 of them
- A list of Issues – Enabling Software is needed
- A word from UKAEA

# A UK Initiative - ExCALIBUR

- **ExCALIBUR** (Exascale Computing Algorithms and Infrastructures Benefitting UK Research) is a £45.7m Strategic Priorities Fund (SPF) programme led by the Met Office, UKAEA 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:
  1. a **knowledge integration** activity;
  2. activities to address **high priority use cases**;
  3. supporting **emerging requirements for high-performance algorithms**;
  4. **cross-cutting research**; and
  5. **proof-of-concept hardware – the Hardware and Enabling Software Programme**.
- UK Research and Innovation expects our first projects to be up and running by April-May 2020.

# 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

# Role of H&ES Programme

- UKRI, Met Office and UKAEA Software Development Calls
  - Create communities of interest around key applications and algorithms
- Hardware and Enabling Software Programme
  - **£4.5M** in capital funding over 4.5 years to develop a hardware foresighting programme.
  - Industry co-funding for the programme will be sought where possible.
  - provide a testbed area that uses pre-commercial equipment for software prototyping and development. It has two main purposes:
    - enable the software community to be ready to use commercial products effectively as soon as they come on to the market;
    - provide the UKRI community with the ability to influence the technology industry and the necessary knowledge to guide their purchase decisions.
- This double-pronged approach will give UK researchers a competitive advantage internationally.

# Benefit and Impacts

**Science delivery:** The work carried out is expected to enhance our exploitation of existing hardware as well as supporting a new Exascale software development roadmap.

**Lower the bar to the ExCALIBUR community to participate in co-design projects with high potential impact.**

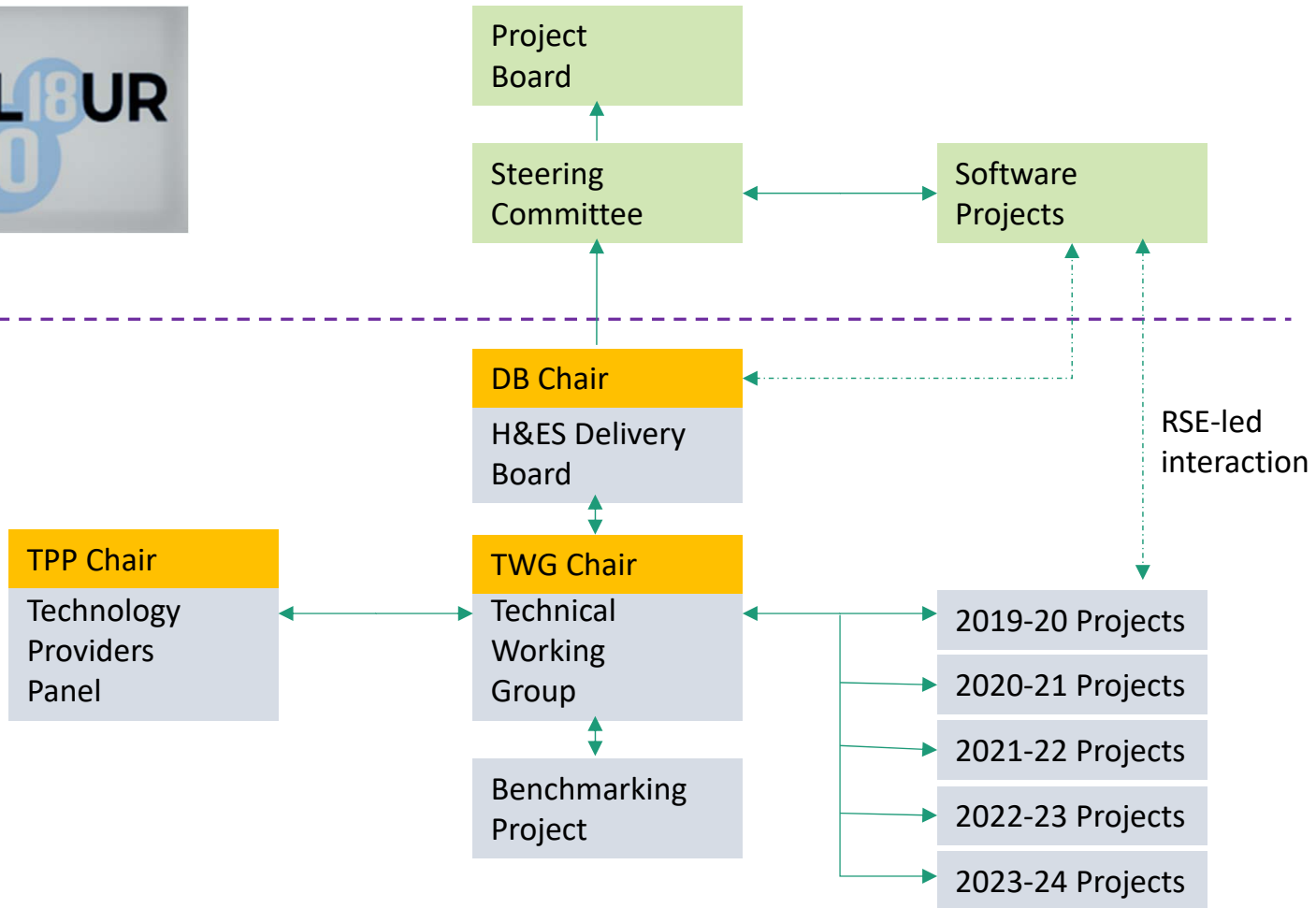
**Prepare for future technology developments** and ensure the ExCALIBUR code base is able to take full advantage of these advances to deliver the science programme.

**Strategic benefit to the ExCALIBUR programme:** this activity formalises ExCALIBUR's continued importance for the delivery of the co-design work needed to prepare for future UKRI HPC services.

- It maintains the confidence of our industry partners and will ensure their continued engagement with ExCALIBUR in the innovation projects which both enhance the current ExCALIBUR science programme and prepare for the deployment of future systems.



Hardware &  
Enabling  
Software



# Benchmarking systems that don't exist yet

- Set ourselves of being able to benchmark systems that don't yet exist.
- We view our systems as analogs (surrogates) for Exascale
- Design new methods to link application performance to system performance
- Make use of
  - Synthetics
  - Mini-apps
  - Applications
- Outputs will be curated



# Separation of Concerns in Practice

- the maths of a problem is separate from its implementation
- So we need Algorithms – the maths made manifest in terms of computational procedures. This leads to
- Co-design; the holistic, collaborative system design by mathematicians, domain scientists, computer scientists and industrial partners
  - The programming language is as much part of the “system design”
- This must deal with new workflows to manage and analyse vast volumes of simulation data
- And round the Loop we go – iterating until we converge
- This requires Investing in People
  - interdisciplinary Research Software Engineer (RSE) career development driven by forward-looking scientific software design
- ResOps – link between software and systems

# A list of Software Working Group Projects

PI	Organisations	Grant Title
<b>Parsons</b>	Edinburgh, Imperial, Exeter, Swansea, Cambridge	ELEMENT - Exascale Mesh Network
<b>Woodley</b>	UCL, Lincoln, Edinburgh, York, Imperial, Cambridge, Oxford, STFC, Turing,	Materials and Molecular Modelling Exascale Design and Development Working Group
<b>Ham</b>	Imperial, Oxford, Exeter, Warwick	Gen X: ExCALIBUR working group on Exascale continuum mechanics through code generation.
<b>Luo &amp; Wells</b>	UCL, Cambridge	Exascale Computing for System-Level Engineering: Design, Optimisation and Resilience
<b>Bower</b>	Durham	Massively Parallel Particle Hydrodynamics for Engineering and Astrophysics
<b>Jeyarajan</b>	STFC, Oxford, UCL	Benchmarking for AI for Science at Exascale (BAISE)
<b>Del Debbio</b>	Edinburgh, Plymouth, Swansea, STFC, Southampton	Lattice Field Theory at the Exascale Frontier
<b>Weinzierl</b>	Durham	ExaClaw: Clawpack-enabled ExaHyPE for heterogeneous hardware
<b>Costanzo,</b>	Sheffield., STFC, Warwick, Imperial	ExCALIBUR-HEP – Data Movement, Organisation and Access
<b>Laizet</b>	Imperial, Southampton, Warwick , STFC, Bristol	Turbulent Flow Simulations at the Exascale: Application to Wind Energy and Green Aviation

## Shallow Dive 1: Gen X: ExCALIBUR working group on Exascale continuum mechanics through code generation.

- Continuous physical systems whose behaviour can be modelled by partial differential equations
- Flow past aircraft and through jet turbines, the propagation of earthquakes, the motion of the weather, the electrical behaviour of the heart and brain, the deformation of a helmet during impact
- Solutions of PDEs – require looking at PDE equations for large scale – do some processes become impossible to solve? Will they need to be pre-conditioned?

# Objectives

- The outer loop: transforming simulation into science
- Data, analysis, and visualisation
- Uncertainty quantification via multi-level Monte Carlo
- Bifurcation analysis via deflation
- Design approach: achieving separation of concerns through composability and code generation
- Building APIs for functions

# Codes and Applications

- Code generation capabilities for extreme-scale PDE discretisation
- Composable outer loop layers for
  - multi-level Monte Carlo for uncertainty quantification,
  - parallel time stepping algorithms,
  - model order reduction,
  - bifurcation analysis of non-linear PDEs,
  - and PDE-constrained optimisation
- Programmable on-line analysis and visualisation
- Deployable software from laptop to supercomputer

Code	
<b>Firedrake</b>	Scales to 25000 Archer cores
<b>OP2 and OPS</b>	<p>Oxford Parallel libraries for Unstructured (OP2) and Structured (OPS) mesh solvers.</p> <p>The separation of concerns enables appropriate optimizations for near-optimal performance on each platform, including SIMD, OpenMP, CUDA, OpenMP4.0, OpenACC, OpenCL combined with MPI.</p> <p>OpenSBLI has been demonstrated to scale up to 98 304 processor cores on ARCHER (over 80% of the machine), up to 256 GPUs on the Cambridge Tier-2 Wilkes2 cluster (over 70% of the machine) and up to 4096 GPUs on ORNL's Titan supercomputer (over 20% of the machine)</p>
<b>PyFR</b>	<p>PyFR is a cross-platform open-source CFD solver that implements the high-order Flux Reconstruction (FR) approach of Huynh for unstructured mixed element meshes.</p> <p>13 PFLOP/s on 18,000 K20X GPUs of Titan (at ORNL)</p>
<b>Devito</b>	<p>Devito is a Domain-Specific Language (DSL) and code generation framework for the finite difference solvers for both forward modelling and PDE constrained optimisation problems such as inversion. Devito allows definition of operators from symbolic equations and generates optimised code specific to a given target architecture. The generated code is parallelised using OpenMP for shared memory parallelism, MPI for distributed memory parallelism and OpenMP offloading for GPUs</p>

# Shallow Dive 2: ELEMENT - Exascale Mesh Network

- computational fluid dynamics, structural engineering, biomechanics and even astrophysics
- Distributed representation of the CAD system
- The high priority use case addressed in ELEMENT is that of meshing for and at the Exascale. Meshes are discrete approximations of real-world domains or geometries. Generating, adapting, partitioning, and visualising meshes efficiently and effectively is therefore a vitally important aspect of any scientific or industrial simulation that models such geometries. ELEMENT will work towards:
  - Meshing for the Exascale: ensuring that meshes are of sufficient quality to represent Exascale problems and can be partitioned efficiently to minimise load imbalance;
  - Meshing at the Exascale: creating highly scalable solutions that will be able to exploit extreme levels of parallelism.



- Serial generation of an initial mesh is no longer viable, this calls for the distributed parallelisation of the whole workflow.
- meshing and geometry management remains a significant bottleneck for complex applications on HPC platforms
- Parallelisation of the mesh generation process
- Automatic mesh sizing and adaptivity
- Fault tolerance
- High-order mesh generation
- Community Building
- Proof of Concept 1 - Scalable Mesh Refinement
- Proof of Concept 2 - Parallel Meshing (EGADSlite)

# Summary of 19-20 & 20-21 H&ES Projects

1. **UCL** for Interconnect Testing, developing the adaptable cluster and developing system-application monitoring methods
2. **UCL** to establish the ExCALIBUR Hub for Hardware and Enabling Software, a training programme and a knowledge transfer activity
3. **Durham** to investigate Exascale solutions for Storage and RAM as Fabric Services, and deploy an AMD test System
4. **Leicester** to characterise the performance of Processor units and attached accelerators and so improve Application performance
5. **Cambridge** to Test and Tune File Systems, Block Storage and Object Stores for Exascale systems
6. **Edinburgh** to Improving application performance by measuring the communication properties for a range of processor unit and accelerator systems; and testing and improving APIs for a range of processor unit and accelerator systems.



# A list of Issues – Enabling Software is needed

- Data Management, Organisation and Access
- “SYCL” type cross-platform abstraction layer for portability to enable code for heterogeneous processors to be written in a “single-source” style using completely standard C++
  - Are they any good?
  - Do they support architectural diversity
- What about MPI
  - That’s the vendors problem isn’t it – well no.....

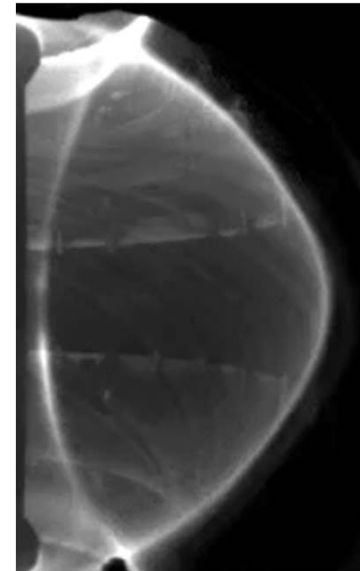
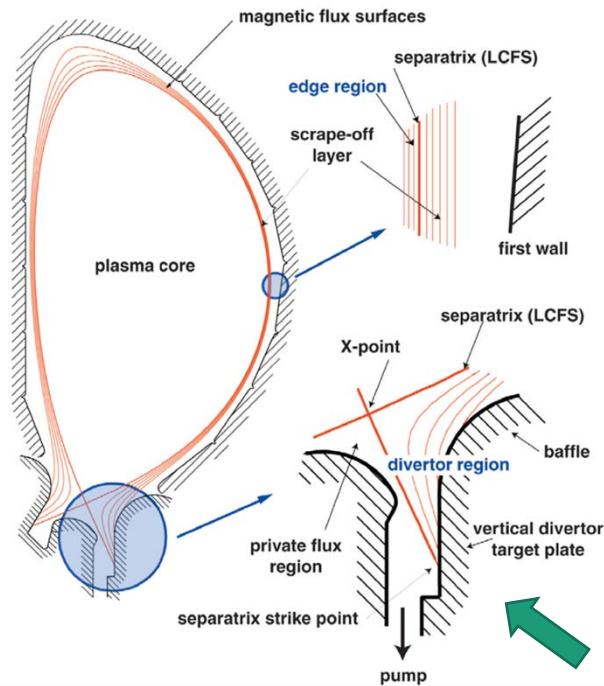
# How we will work with you

- RSE/ResOPs with each project, which is the main interface with a Software Project
- Benchmarking is a key activity – Andy Turner is our co-Ordinator.
  - Synthetics
  - Mini-apps
  - Applications
- Make ARMFORGE available to projects
- Ask you what technologies you would like to use now
  - View our systems as analogs (surrogates)
- What would you like to see put in place.
- Sort out routes

# Fusion Modelling System Use Case

(NEPTUNE : NEutrals & Plasma TUrbulence Numerics for the Exascale)

MAST: UK's EPSRC programme Tokamak



Challenging, coupled multi-physics problem

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Aim: create new knowledge, skills and tools leading to the instantiation of an Exascale scalable infrastructure for modelling the complex physics of the tokamak plasma edge

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# 7 planned Calls imminent

**Y1 activities are all “exploratory” through the development of “Proxyapps”:**

- 1. Numerical representation - Performance of Spectral Elements**
- 2. Numerical representation - Optimal Use of Particles**
- 3. Numerical representation - Study of uncertainty quantification (UQ) techniques**
- 4. Numerical representation - Study of Model Order Reduction (MOR) Techniques**
- 5. Numerical representation - Investigate matrix-preconditioning techniques**
- 6. Development of Edge Plasma Fluid Referent Model**
- 7. Development of Gyro/Drift Kinetic Referent Model for Plasma Edge**





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Thank you



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