ExCALIBUR Programme aims:
Radical changes to supercomputer architectures are on the horizon. The current simulation codes, that much of UK science relies on, are designed for current supercomputer architectures. These codes will, at best, not be able to fully exploit the power that the supercomputers of the mid-2020s will deliver; at worst, they will run slower on those machines than they do now. Future computers will be more energy efficient and so the longer we rely on the current approach, the more expensive the solution will be. Therefore, it is essential that we invest now in redesigning those simulation codes so that they perform well on the future generations of supercomputers.

ExCALIBUR will meet this challenge by delivering research and innovative algorithmic development to redesign the high priority simulation codes to fully harness the power of future supercomputers across scientific and engineering applications. It will achieve this by bringing together an unprecedented range of UK domain experts, mathematicians and computational scientists who will identify common issues and opportunities in the high priority simulation codes and focus their combined scientific expertise and resources to accelerate toward interdisciplinary solutions.

The programme objectives have been designed to specifically address the benefits sought:
1. **Efficiency** - The UK's most important scientific simulation codes will be able to harness the power of the supercomputers of the mid-2020s resulting in an increase in scientific productivity for a given investment.
2. **Capability –** Capitalising on this efficiency will enable the UK to continue to push the boundaries of science across a wide range of fields delivering transformational change in capability.
3. **Expertise** – A new, forward-facing, interdisciplinary approach to RSE career development will position the next generation of UK software engineers at the cutting-edge of scientific supercomputing.

ExCALIBUR is built around four pillars: separation of concerns; co-design; data science; and investing in people. These pillars describe the fundamental principles that guide the development of research under ExCALIBUR and are designed to ensure that the outcomes are future proofed against the constantly evolving landscape of hardware design. It will be delivered through six main activities: the redesign of a core set of simulation codes (use cases) chosen to span a wide range of science domains; knowledge integration across the programme through widely applicable cross-cutting themes; application of learning from these activities to a second wave of use cases; exploratory research to identify and develop emerging high-performance algorithms in areas with significant potential impact; an interdisciplinary Research Software Engineer knowledge integration activity; and an annual capital investment to support the development of novel test beds to enable co-development with industry.

ExCALIBUR Cross-Cutting Themes:
A key element of the delivery of the ExCALIBUR Programme is the development of cross-cutting themes and associated activities that apply across Use Cases. These will be funded by the SPF ExCALIBUR Programme partners, the Met Office and EPSRC they will incorporate the topics listed below. All of these calls are for a three year duration and are complementary so please do consider which call would be best for your submission.

The output of each activity should be applicable to at least two out of: the Weather & Climate Prediction Use Case; the Fusion Modelling Use Case; and any collection of the Design &

Development Working Group Use Cases. Code should be developed for one of these and a report prepared on the applicability to one or more of the others.

Cross Cutting Work Package 1 "Common approaches and solutions"
The activities of this work package will explore and accelerate the development of solutions and approaches to problems that are common to more than one use case and that will thereby enhance the ability of the community to better exploit exascale computing power.

- **I/O & storage *(Met Office led)***

Development and demonstration of novel approaches to optimising aspects of the data flow through the memory hierarchy which will help alleviate the increasingly important I/O bottleneck for practical large-scale applications.

- **Data workflow *(Met Office led)***

Development and demonstration of novel approaches to taking certain computations to the data which will help reduce the need for expensive data movements and thereby help alleviate the increasingly important I/O bottleneck for practical large-scale applications.

- ***Coupling (EPSRC led)***

Applicants to submit proposals that investigate and research coupling technologies that address the complexity of concurrently running multiple applications required to produce unified results for heterogeneous systems.

- ***Domain Specific Languages (EPSRC led)***

Various existing and upcoming programming languages are utilised or under development, requiring some standardisation as we move towards Exascale. Proposals to provide solutions that drive efficient practices for Exascale; identify resolutions of barriers for co-design across domain-specific languages or consider interoperability between languages. Applicants should consider how they will integrate and optimise their findings parallel with the scientific code development by the ExCALIBUR Use Cases.

Cross Cutting Work Package 2 "Potential Disruptors"
The activities of this work package will explore, and accelerate the development of such new, potentially disruptive, technologies that will enhance the ability of the community to better exploit exascale computing power. Each will deliver the following:

- ***Exposing parallelism: Parallel-in-Time (Met Office led)***

A roadmap for how use-case applications can adopt parallel-in-time approaches; a standard set of appropriate and challenging test cases to demonstrate the efficacy of parallel-in-time approaches; and an environment that allows the rapid prototyping of a variety of methods and benchmarking of those test cases.

- ***Exposing parallelism: Task Parallelism (Met Office led)***

A review of the potential for practical application of task-based parallelism to various use cases; an investigation of methods for abstracting aspects of task-based parallelism that could be interfaced to generic engines or to relevant domain specific languages; and a prototype implementation of this abstraction and its application to the relevant use cases.

- ***ML: optimising numerical methods & augmenting physically based applications (Met Office led)***

A standardised approach, either via libraries or interfaces, to the fusion of a range of machine learning tools and simulation codes representing the relevant use cases that will facilitate the uptake of ML methods to improve and optimise existing numerical methods and physically based simulations.

- ***Future Computing Paradigms (EPSRC led)***

Proposals within this theme must be potential disruptors to the current practices within the development and optimisation of Exascale software and architecture. Potential disruptors include, but are not limited to Quantum technology, Artificial intelligence and Neuromorphic computing. These approaches may simulate future Exascale systems, management of vast amounts of data or mixed-precision performance.

- ***Verification, Validation and Uncertainty Quantification (EPSRC led)***

Proposals within this theme are required to develop and implement Verification, Validation and Uncertainty Quantification (VVUQ) parameters for Exascale. VVUQ is essential to establishing actionable and trusted software for future systems and will enable integration across the ExCALIBUR Programme, specifically with Use Cases.

Applicants to EPSRC led calls to complete an Intent to Submit survey to indicate their interest in this upcoming call. The survey will go live in February 2021. Please send enquiries to researchinfrastructure@epsrc.ukri.org in the interim.

For Met Office led calls please see details on our website: Opportunities - Met Office