



## November 2020 newsletter - Strategic Priorities Fund (SPF) ExCALIBUR programme

Welcome to this ExCALIBUR newsletter, in which we hope to bring you up to date with the progress being made in the programme.

If you have been forwarded this newsletter and would like to receive future issues direct, please [email us](#) with your details and to provide your consent.

### Cross-cutting themes engagement activity

We are pleased to inform you that the ExCALIBUR programme will be launching an engagement activity during the week commencing 16 November 2020. This activity will be in the form of an online presentation to provide an opportunity for engagement with UK academia and relevant organisations in developing cross-cutting themes and will aid us in the development of the future funding calls. The web link to this event will be circulated the week of 16 November and will be live for two weeks (deadline 04 December at 12 noon). Viewers will be invited to complete a response form to capture their ideas and suggestions to aid the development of the forthcoming calls. Guidance and further information will be included on the web page and we look forward to hearing your ideas and suggestions. The calls are expected to launch at the beginning of 2021 and will be delivered by the Met Office and EPSRC; the resulting grants are anticipated to begin in June 2021.

### Fusion modelling use case

The series of eight calls under Project NEPTUNE (Neutrals & Plasma TURbulence Numerics for the Exascale) recently closed and awards are expected to be announced in early 2021. Project NEPTUNE seeks to develop knowledge, capability and prototype infrastructure targeting one of the Grand Challenge problems in modelling the behaviour of a thermonuclear plasma – the so-called “tokamak edge”, where hot plasma interacts with cooler neutral atoms and the machine wall itself. The system of equations forms a classic multi-physics, multi-scale Grand Challenge problem that has long been heralded as “Exascale class” and as such, requires a UK wide team in order to build an “actionable” platform targeting ITER (a €25B reactor class tokamak being constructed in the South of France) and for designing the world’s first commercial fusion reactors (for the example of the UKAEA-led STEP programme, an ambitious project to deliver fusion power to the grid in the 2040’s, click [here](#)). Initial activities are designed to form an “exploratory phase” and to build a UK wide community around the project.

### Weather and climate use case

The weather and climate use case has commissioned the UK Chemistry & Aerosol (UKCA) activity to the University of Cambridge. The aims of this activity are: to create a functioning stand-alone version of the UKCA model with its own driver, in an appropriate repository, and with its own testing strategy; deliver an analysis of the bottlenecks and hindrances to improved performance of UKCA on current and anticipated supercomputer architectures; recommend how to address those bottlenecks and hindrances; and implement and test the most important modifications to deliver, with demonstration, a significant improvement in UKCA performance and flexibility. In October the Met Office started work on a coupling activity which aims to deliver the option of a new paradigm within the UK's weather and climate prediction system for coupling together the ocean and atmosphere modelling components as a single executable. This will provide the flexibility to optimise the data flow of the coupled system for whatever the future hardware systems look like. This will be essential to enable optimal and flexible use of those future systems. It is also anticipated that learning from this activity will inform a broader ExCALIBUR cross-cutting activity in coupling and couplers.

## UKRI high priority use case

Ten Design and Development groups (DDWGs) were awarded in April 2020 to conduct a mixture of simulation code design and development, and community building activities that will engage relevant computational and user communities, addressing the 'high priority use case' theme within the ExCALIBUR programme.

A kick-off workshop was held in July 2020 on behalf of UKRI, the Met Office, and UKAEA for the DDWGs members and Steering Committee members. To promote collaborative working between DDWGs, topics of discussion were the cross-cutting themes within the programme and an opportunity for groups to discuss commonalities or differences in their research.

DDWGs have been hosting community workshops for their use cases since the summer. Recently some of these groups held workshops or have them planned for the near future. **Exascale SLE** and **ELEMENT** have hosted workshops with international participants in September and October respectively, and **GenX** will host a workshop on 24-25 November. Further workshops and events are anticipated from the remaining groups. Each of the funded projects can be found [here](#).

For more information on this activity please contact: [Billy McGregor](#)

## UKRI Hardware and Enabling Software (H&ES) Group

The annual capital investment supports development of novel test beds to enable co-development with industry. This investment will be used to support the deployment of a number of innovative proof-of-concept systems. As well as providing early testing of solutions on potential future architectures, a crucial aspect is that these systems will also test the suitability of new hardware for deployment at scale within national computing services. These systems are available to ExCALIBUR partners and wider scientific communities, with a particular emphasis on the UKRI software use-case groups.

H&ES launched their annual call in 14 September 2020 to host hardware for the wider community and expects to fund 4-5 projects each year; outcomes of recent submissions will be known by 30 December 2020. Further information on the call and scope of the H&ES can be found on their [website](#).

## Research Software Engineer Knowledge Integration

Calls associated with this activity are not scheduled until next year. Currently the DDWGs are tasked with developing a landscape review of the training and skills requirements of Research Software Engineers (RSE)

in preparation for Exascale systems. A proportion of the groups will also identify, prepare and deliver training and upskilling of the current RSE community.

For more information on this activity please contact: [Sarah King](#)

## Steering Committee

The **ExCALIBUR Steering Committee** held its second virtual meeting on 9 October 2020 where members discussed stakeholder engagement plans, development of the cross-cutting themes and how to increase interdisciplinary activities within the programme.

## ExCALIBUR programme website

A website for the ExCALIBUR programme is being created and will be launched in early 2021. This will provide key information on the progress of the programme and will be a repository for key documentation for dissemination of the ExCALIBUR benefits and outcomes.

## The Exascale Computing Algorithms and Infrastructures Benefiting UK Research (ExCALIBUR) programme

ExCALIBUR is a programme within the UK Research and Innovation (UKRI) Strategic Priorities Fund (SPF) with total funding of £46m from October 2019 to March 2025. It is delivered in partnership between UKRI Research Councils (led by the Engineering and Physical Sciences Research Council (EPSRC)) and the department for Business, Energy and Industrial Strategy (BEIS) Public Sector Research Establishments (PSRE) (led by the Met Office).



ExCALIBUR is delivering research and innovative algorithmic development to redesign the UK's high priority simulation codes to fully harness the power of future supercomputers across scientific and engineering applications. (Such computers are referred to as Exascale since they are targeting delivering a billion billion floating point operations a second and a similar amount of data). It is committed to bringing together an unprecedented range of UK domain/subject-matter experts, mathematicians and computational scientists who will identify common issues and opportunities 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:

- **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.
- **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.

- **Expertise** – A new, forward-facing, interdisciplinary approach to Research Software Engineer (RSE) career development will position the next generation of UK software engineers at the cutting-edge of scientific supercomputing.

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