



Quick Reference

ExCALIBUR High Priority Use Cases: Phase 1 (Design & Development Working Groups)

Call type: Invitation for proposals

Closing date: 22 January 2020 at 16:00

Funding Available: Up to £1.2m to support 4-8 working groups for 15 months

How to apply: Full proposals.

Assessment Process: proposals will be considered by an expert panel, resulting in a rank ordered list. There will be no postal peer-review stage.

Key Dates:

Activity	Date
Call opening date	27 November 2019
Call closing date	22 January 2020
Expert panel	Week Beginning 24 February 2020
Funding decision	March 2020
Grant start date	01 April 2020
Grant end date	31 June 2021

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UK Research
and Innovation

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Call type: Invitation for proposals

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Related themes: Research infrastructure

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Summary

ExCALIBUR (Exascale Computing Algorithms and Infrastructures Benefitting UK Research) is a £45.7m Strategic Priorities Fund (SPF) programme led by the Met Office and UK Research and Innovation to meet this challenge by delivering research and innovative algorithmic development to harness the power of exascale HPC.¹

As part of this wider project, UK Research and Innovation is seeking proposals for multi-disciplinary Design and Development Working Groups to undertake a

¹ <https://www.gov.uk/government/news/88-million-to-help-unleash-the-productive-power-of-the-uk-economy>

programme of activities to develop software for the anticipated deployment of exascale systems in the mid-2020s. Design and Development Working Groups will bring together a wide range of domain experts, mathematicians, computational scientists, and Research Software Engineers (RSEs) 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.

Background

The ExCALIBUR programme

Radical changes to High Performance Computer (HPC) architectures are on the horizon, in order to enable the transition from petascale to exascale levels of performance. Exascale systems have the potential to make dramatic impacts in multiple disciplines, including – but not limited to – materials science, medical research, energy, genomics, particle physics and engineering. However, the full capability of exascale computing cannot be effectively exploited without appropriate software: existing simulation codes will not perform effectively on exascale systems.

ExCALIBUR (Exascale Computing Algorithms and Infrastructures Benefitting UK Research) is a £45.7m Strategic Priorities Fund (SPF) programme led by the Met Office and UK Research and Innovation to meet this challenge by delivering research and innovative algorithmic development to harness the power of exascale HPC.²

ExCALIBUR will be delivered over five years through a suite of complementary activities: a knowledge integration activity between software engineers (£0.75 million); high priority use case activities, which will be developed through a mixture of open calls, commissioned research and single tenders (£5-7 million each); a second wave of use cases (~£2 million each); funding for disciplines with emerging requirements for high-performance algorithms (£3 million); cross-cutting research activities to drive impact (£10 million); and capital funds to develop proof-of-concept systems with new computer architectures in partnership with industry (£4.5 million).

The ExCALIBUR approach is based around four pillars:

1. **Separation of Concerns:** the maths of problem is separated from the computer science of implementation;
2. **Co-design:** holistic, collaborative system design by mathematicians, domain scientists and computer scientists;
3. **Data Science:** new workflows to manage and analyse vast volumes of simulation data; and
4. **Investing in People:** interdisciplinary Research Software Engineer (RSE) career development driven by forward-looking scientific software design.

² <https://www.gov.uk/government/news/88-million-to-help-unleash-the-productive-power-of-the-uk-economy>

Scope

This UK Research and Innovation call for proposals, led by EPSRC, addresses the 'high priority use case' theme within the ExCALIBUR programme and is informed by the outputs of a scoping workshop held on 27 June 2019 in London. It is complementary to a parallel programme of activities led by the Met Office and the UK Atomic Energy Authority to address high priority use cases in the areas of weather and climate prediction, and fusion modelling, respectively.

Accordingly, applicants working in any field of research supported by UK Research and Innovation are invited to apply. However, **proposals focussed on weather and climate modelling and fusion modelling are out of the scope of this call and will not be accepted.**

The UK Research and Innovation contribution to the high priority use case theme will be delivered in three phases:

1. **Phase 1** (this call): up to £1.2m to support 4-8 Design and Development Working Groups for 15 months. Design and Development Working Groups will bring together a wide range of subject matter experts, RSEs, computational and/or mathematical scientists, and any other relevant individuals and groups, to design and develop simulation codes for exascale computing can be applied by a wide range of users in strategically important areas of research.
2. **Phase 2**: after 12 months of operation, the Design and Development Working Groups will be reviewed by an independent expert panel to determine their progress against the objectives of this call. This review will assess the individual performance of Working Groups, as well as their collective performance as a collaborative network. Following the review, successful Working Groups will be provided with the opportunity to secure further funding for research and development projects. Guided by the findings of the evaluation panel, UK Research and Innovation may make further funding conditional on the reconfiguration of working groups, including changes to their composition and work plans. At this stage, there will be opportunities for new entrants to apply to participate in research and development projects.
3. **Phase 3**: a second wave of use case calls will be launched at a later stage.

The objectives of Design and Development Working Groups are to foster communities of practice that will progress simulation code design and development activities for exascale computing in accordance with the four pillars that define the ExCALIBUR approach (described above).

Design and Development Working Groups must address **high priority use cases**. We define a high priority use case as having the following characteristics:

- Enables high quality, high impact research in multiple areas of strategic importance;
- Provides 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;

- Provides a national and international focal point for the relevant research communities, including the development of partnerships with complementary initiatives in the UK and internationally.

In order to address high priority use cases, Design and Development Working Groups are expected to develop a coherent community of practice comprising subject matter experts, RSEs, computational and/or mathematical scientists, and any other relevant individuals and groups. The composition of a Working Group should be appropriate in scale and expertise to the design and development programme being proposed. It should enable effective engagement between the computational research community and research communities that can benefit from exascale computing.

Design and Development Working Groups will be expected to collaborate with other Working Groups in order to develop cross-cutting approaches to common computational elements³ that have relevance to multiple codes and applications. A kick-off workshop will be organised by UK Research and Innovation at the start of the awards to facilitate collaborative working between Working Groups, the Met Office, UK Research and Innovation and the UK Atomic Energy Authority. Applicants should ensure that sufficient funding is requested to progress cross-cutting topics of mutual interest for the duration of the award.

Outputs and outcomes

Working Groups are expected to conduct a mixture of simulation code design and development, and community building activities that will engage relevant computational and user communities. The proposed approach should be consistent with the four pillars of the ExCALIBUR programme and should include cross-cutting approaches to common computational elements that have relevance to multiple codes and applications.

Working Groups are expected to deliver, *inter alia*, the following outputs:

- A strategic research agenda that clearly articulates the research challenges to be overcome, opportunities, key risks and mitigations, and sets out a detailed approach to addressing these to enable development of exascale-ready software by the mid-2020s.
- Evidence that the proposed approach has been developed collaboratively with potential beneficiaries, including co-design with industry where appropriate.
- Demonstration of the feasibility of the proposed approach through proof-of-concept studies and research outputs. Scaling should already be demonstrated at the petascale and relevant software development should already be underway.⁴

³ Similar approaches have been adopted by the Exascale Computing Project in the US, an activity jointly sponsored by the US DOE Office of Science and the National Nuclear Security Administration. <https://www.exascaleproject.org/>

⁴ For groups that are not at this stage there will be further opportunities in later stages of the wider ExCALIBUR project.

Funding available

Up to £1.2m will be available to fund four to eight working groups (i.e. £150k - 300k per proposal). The duration of the proposals should be 15 months from 01 April 2020.

Equality, Diversity and Inclusion

The long term strength of the UK research base depends on harnessing all the available talent. EPSRC expects that equality and diversity is embedded at all levels and in all aspects of research practice and funding policy. We are committed to supporting the research community, offering a range of flexible options which allow applicants to design a package that fits their research goals, career and personal circumstances. This includes career breaks, support for people with caring responsibilities, flexible working and alternative working patterns. With this in mind, we welcome applications from academics who job share, have a part-time contract, or need flexible working arrangements.

Peer review is central to EPSRC funding decisions, we require expert advice and robust decision making processes for all EPSRC funding initiatives. We are committed to ensuring that fairness is fully reflected in all our funding processes by advancing policy which supports equality, diversity and inclusion. Please see our Equality and Diversity webpages

<https://epsrc.ukri.org/funding/equalitydiversity/> for further information.

Guidance on Journal-based metrics

As part of our commitment to support the recommendations and principles set out by the San Francisco Declaration on Research Assessment (DORA; <https://sfdora.org/read/>), UK Research and Innovation reviewers and panel members are advised not to use journal-based metrics, such as journal impact factors, as a surrogate measure of the quality of individual research articles, to assess an investigator's contributions, or to make funding decisions.

The content of a paper is more important than publication metrics, or the identity of the journal, in which it was published, especially for early-stage researchers. Reviewers and panel members are encouraged to consider the value and impact of all research outputs (including datasets, software, inventions, patents, preprints, other commercial activities, etc.) in addition to research publications. We advise our peer reviewers and panel members to consider a broad range of impact measures including qualitative indicators of research impact, such as influence on policy and practice.

Equipment

Equipment over £10,000 in value (inc. VAT) is not available through this call. Smaller items of equipment (individually under £10,000 inc. VAT) should be in the Directly Incurred - Other Costs heading.

For more information on equipment funding, please see:

<https://epsrc.ukri.org/research/facilities/equipment/>

Eligibility

The PI and any Co-Is should have Investigator level registered Je-S accounts. Please allow at least two weeks to create Je-S accounts for Investigators who do not currently have one.

For information on the eligibility of organisations and individuals to receive UK Research and Innovation funding, see: <https://www.ukri.org/funding/how-to-apply/eligibility/>

How to apply

Submitting an application

You should prepare and submit your proposal using the Joint electronic Submission (Je-S) System (<https://je-s.rcuk.ac.uk/>).

When adding a new proposal, you should select:

- Council 'EPSRC'
- Document type 'Standard Proposal'
- Scheme 'Standard'
- On the Project Details page you should select the 'Software use code development for exascale computing' call.

Note that clicking 'submit document' on your proposal form in Je-S initially submits the proposal to your host organisation's administration, not to EPSRC. Please allow sufficient time for your organisation's submission process between submitting your proposal to them and the call closing date. EPSRC must receive your application by 16:00 on 24 January 2020.

Guidance on the types of support that may be sought and advice on the completion of the research proposal forms are given on the EPSRC website (<https://epsrc.ukri.org/funding/applicationprocess/>) which should be consulted when preparing all proposals.

Guidance on writing an application

Proposals will have a start date of 01 April 2020 and a fixed duration of 15 months. As well as the standard call form, applicants should submit the following documents in support of their application.

Case for Support (up to 8 pages) including:

Track record of the PI and Co-Is contributing to the project (2 pages), indicating how their expertise will contribute to the overall composition of the Working Group.

Case for Support (6 pages) including:

- Detailed description of how the proposed Working Group contributes to the aims and objectives of this call, and why the proposed Working Group will advance the current state-of-the-art.
- The focus area of the proposed Working Group and the challenge(s) to be addressed. Technical details of the approach to the design and development of simulation code(s) should be included.
- The timeliness and importance of the proposed Working Group and the potential for leverage and/or collaborative activity.
- Description of the planned proof-of-concept activities, approach to community development, and engagement activities.

Pathways to Impact (up to 2 sides of A4)

Please provide a short statement on the anticipated impact of your proposed investment, who will be the likely beneficiaries and how you propose to engage with them in order to ensure your outputs are fit for purpose and benefits have the potential to be maximised.

Work Plan (up to 1 side of A4)

This should include details of the timescales for the planned activities.

Justification of Resources (up to 2 sides of A4)

Please ensure that all items requested on the Je-S form are fully justified.

CVs (up to 2 sides of A4 each):

For named researchers, RSEs or visiting researchers only, not the PI or Co-Is.

Project Partner Letters of Support (no page limit)

A statement of support must be attached for every project partner identified; only one letter is allowed per organisation. Each letter must be on headed paper, signed, and dated within 6 months of the application date to EPSRC.

Project partners must be making a contribution to the proposal which should have an approximate financial value attached to it. At the same time they should not be receiving money from the grant.

The host organisation(s) of the PI or Co-I cannot be a project partner.

Letters of Support (no page limit)

Letters of support from interested parties who are not project partners can be added to the proposal. A maximum of three letters of support per application will be allowed. Letters should provide a substantial explanation of the value of the proposed work and how this is relevant to their organisation. Each letter must be on headed paper, signed, and dated within 6 months of the application date to EPSRC.

Applicants should use the Ethical Information section on the Je-S form to demonstrate to peer reviewers that they have fully considered any ethical issues

concerning the material they intend to use, the nature and choice, current public perceptions and attitudes towards the subject matter or research area. EPSRC will not fund a project if it believes that there are ethical concerns that have been overlooked or not appropriately accounted for. All relevant parts of the Ethical Information section must be completed. If the research will involve human participation or the use of animals covered by the Animals (Scientific Procedures) Act 1986 it is recommended that applicants pay particular attention to the guidance highlighted below. EPSRC reserves the right to reject applications prior to peer review if the Ethical Information sections are not completed correctly.

Further guidance on completing the Je-S form can be found at <https://je-s.rcuk.ac.uk/Handbook/pages/GuidanceonCompletingaStandardG/EthicalInformation.htm>. Other relevant guidance includes: EPSRC's policy on animal use in research (<https://www.epsrc.ukri.org/about/standards/animalresearchpolicy/>) and the Responsible Innovation Framework (<https://epsrc.ukri.org/research/framework/>).

Please note that on submission to EPSRC **all** non-PDF documents uploaded onto Je-S are converted to PDF, the use of non-standard fonts may result in errors or font conversion, which could affect the overall length of the document.

For advice on writing proposals see:

<https://epsrc.ukri.org/funding/howtoapply/preparing/>

User Engagement Strategy

Successful applicants will be required to develop and execute a strategy for engaging with relevant groups, including potential future users of the codes whose development would be assisted through the project. Resources for this activity can be requested as part of the Pathways to Impact and must be justified in the application. This strategy should be reviewed and updated regularly as part of the formal management of the grant.

The strategy should cover:

- how and when potential users have been / will be identified;
- what form the engagement will take; how the outputs of the engagement inform development of the codes proposed
- what steps will be taken to ensure that outputs of the research will have the potential to be of value to (potentially multiple) end users;
- suitable metrics for determining the success of the strategy in delivering value to users.

Assessment

Assessment process

There will be no postal peer review stage for proposals submitted to this call. Applications will be assessed by an expert panel.

Assessment criteria

Proposals will be assessed on the following criteria:

- **Quality** (primary): evidence of:
 - the contribution of the proposed Working Group to the ExCALIBUR programme's objective to deliver research and innovative algorithmic development to harness the power of exascale HPC according to the four pillars of Separation of Concerns, Co-Design, Data Science and Investing in People;
 - the contribution of the proposed Working Group to addressing a high priority use case; and
 - the contribution of the proposed Working Group to building a coherent community of practice comprising subject matter experts, RSEs, computational and/or mathematical scientists, as well as any other relevant individuals and groups.

- **Timeliness and feasibility** (secondary major): evidence that:
 - the focus of the proposed Working Group addresses a clear and timely need within the relevant research communities that builds upon existing approaches and has potential to leverage complementary expertise and activities; and
 - the proposed approach of simulation code design and development, and community building activities is feasible within the funding period (will deliver the expected outputs and outcomes).

- **Applicants** (secondary): evidence that the applicants represent the range of disciplines and expertise required to address the challenge described and that the Working Group will be credible to the wider research community.

- **Impact** (secondary) evidence of a credible approach to engagement with relevant research and user communities, including mechanisms to enable co-design.

- **Resources and management** (secondary): evidence that the requested resources and approach to management are appropriate with respect to the activities of the proposed Working Group.

Feedback

As this call will operate a single stage expert assessment process with no postal refereeing stage, applicants will not have the opportunity to respond to the comments of the panel prior to a decision being made. Feedback will not be provided unless the panel requests that specific issues are communicated to the applicants.

Grant additional conditions (GACs)

Grants will be subject to the standard UK Research and Innovation grant conditions. UK Research and Innovation reserves the right to add additional grant conditions prior to award.

Repeatedly Unsuccessful Applicants Policy Submissions to this call will count towards the Repeatedly Unsuccessful Applicants Policy. Further information about the policy can be found at:

<https://epsrc.ukri.org/funding/howtoapply/basics/resubpol/rua/>

Key dates

Activity	Date
Call opening date	27 November 2019
Call closing date	22 January 2020
Expert panel	Week Beginning 24 February 2020
Funding decision	March 2020
Grant start date	01 April 2020
Grant end date	31 June 2021

EPSRC aims to adhere to the key dates as published, however there may be exceptions where the sift, prioritisation or interview meeting may have to change due to panel member availability.

Contacts

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Change log

Name	Date	Version	Change
Antony Chapman	06/08/2019	0.1	N/A
Richard Gunn	20/08/19	0.2	Revisions

Name	Date	Version	Change
Antony Chapman	21/08/19	0.3	Revisions
Antony Chapman	16/10/19	0.4	Revisions following input from UKRI Delivery Group.
Richard Gunn	12/11/19	0.5	Revisions to scope, assessment criteria, and applicant guidance. Inclusion of background to SPF programme. Content and style edits.
Richard Gunn	25/11/19	0.6	Minor style edits.

Je-S attachments Check List

Standard:

Attachment Type	Maximum Page length	Mandatory/Optional	Extra Guidance
Case for Support	Eight pages	M	Comprising up to two A4 sides for a track record, and six A4 sides describing the proposed research and its context.
Pathways to Impact	Two pages	M	
Workplan	One page	M	
Justification for Resources	Two pages	M	
CVs	Two pages each	As Required in the call	For named and visiting researchers, and researcher co-investigators only.
Project Partner Letters of Support	No page limits	As Required in the call	Must be included from all named project partners. Must be on headed paper, and be signed and dated within six months of the

			proposal submission date.
Letters of Support	No page limits	As Required in the call	In exceptional circumstances a maximum of three letters can be submitted.
Technical assessment	No page limit	As required in the call	
Proposal Cover Letter	No page limit	Optional	The cover letter can be used to highlight any important information to EPSRC. This attachment type is not seen by reviewers or panel members.
Other attachment	No page limit	As required; request only	This can be used for a document that does not fit under any of the headings above. This attachment type is not seen by reviewers or panel members.

Please ensure you adhere to the above attachment requirements when submitting your proposal. Any missing, over length or unnecessary attachments may result in your proposal being rejected.