Application Guidance for GPU embedded CSE

Please follow this guidance to help prepare your application for an eCSE call. Proposals should be submitted on-line using the eCSE Funding Calls section within the SAFE (https://safe.epcc.ed.ac.uk/). If you are not a registered SAFE user, please register there first to begin a proposal. Each call has its own proposal form and guidance (this document) and applicants must use the forms associated with the relevant call. Proposals will not be accepted if incorrect forms are used.

The GPU eCSE programme is administered by EPCC through ARCHER2, the UK National HPC Service. However, applications are not limited to projects targeting the GPU component of ARCHER2. Projects may utilise other GPU resources within the UK digital research infrastructure. The call is open to research across all of UKRI's remit.

If your eCSE proposal is selected for funding, you will be provided with an award letter and will be asked to agree to the eCSE Terms. Please view these here:

https://www.archer2.ac.uk/ecse/Terms/ARCHER2_eCSE_Terms.pdf

It is important that you are aware of the Trusted Research policy of your own institution. Information on UKRI's Trusted Research Principles is given here:

https://www.ukri.org/wp-content/uploads/2021/08/UKRI-170821-TrustedResearchandInnovationPrinciples.pdf

Where projects have international partners (e.g. a Co-I from a non-UK institution) we will contact you if your proposal is accepted to ensure that you are aware of, and have read, your own institution's policy and you will need to provide a link to where the information can be found.

I.   Important Information for eCSE Applicants

To be considered for this call, the entire proposal must be submitted in the SAFE by **16:00 on 19 March 2024**. As well as the completed on-line form, this submission should include PDFs of the main proposal document, any costing documents (see below) and letters of support (optional). In addition, any participants in the project (PI, Co-I(s), or technical staff) must have been invited and have accepted the invitation to join the project within the SAFE and added information about their roles within the project and relevant experience. Technical staff should also add a CV. **You will not be able to submit the form if the technical staff have not accepted the invitation**.

Immediately following the closing of the call on the 19 March 2024, proposals will be passed on for review by the eCSE Panel and any missing documents or team members will not be considered to be part of the submission. Costing documents are

required for all members of technical staff and must be submitted when the proposal is submitted.

II.   *Initiating an eCSE Proposal*

First log in to the ARCHER2 SAFE and click on "Funding Calls" under the "eCSE Funding" heading at the top. At the bottom of the page you should see a "New Funding Application" button. Click on this to begin the process of creating an eCSE application. To start an application you should give the project title. You should also choose the subject area of the proposal and choose the most appropriate UKRI research area. In cases where several apply, please pick the most relevant.

Details of the various Research Councils within UKRI are given here:

https://www.ukri.org/councils/

III.   *On-line submission for eCSE application*

The information in this section is aimed at guiding you through completing the on-line form in the ARCHER2 SAFE and associated document

Please give a short summary of your project. This should include enough background description to justify the Research Council remit selected above.

Principal Investigator

Co-Investigators

Members

In these sections, additional project members can be added to the project team by invitation, whereupon their roles can be assigned. All roles have permission to edit the proposal. Allowed roles are:

- PI (leader of the project)
- Co-I (other members of the team who will help to lead or advise on the project)
- Technical Staff (the person or people who will be funded to work on the project)
- Contact (someone working on behalf of the PI who should receive any correspondence – note PIs, Co-Is and technical staff will all receive correspondence automatically so there is no need to give them the Contact role)
- Member (no specific role in the project but can see and edit the proposal)

It is possible to select more than one role for a person and roles can be changed at any time up to the final submission.

The eCSE programme funds staff costs for the technical members of staff. Details of how to cost this are provided later in this document. The programme does not fund PI and Co-I staffing time.

In some cases the PDRA or RSE to be funded to carry out the technical work (with the project role Technical Staff) may have the skills in place to also act as a Co-I or even take on the role of PI. In the latter case it will need to be clear that suitable support is in place within the team (e.g. other members with suitable experience taking on Co-I roles and with at least one of these Co-Is coming from the same institution as the PI). The reason this is allowed is to enable a PDRA or RSE early on in their career to get experience of the more senior PI or Co-I role; however it is not intended as a way of funding the Co-I or PI role or as a way to fund sabbaticals for senior academic staff. There may be cases where a more senior member of staff may be PI or Co-I and may need to take on a small amount of the technical work of the project. If so, they would be funded and costed for this technical work in the same way as any other Technical Staff member and should include a costing breakdown for this work and their CV. An explanation of why this is required should be given in the proposal, and this should not be used as a way of funding the Co-I or PI role.

When inviting another team member, please use the email address that this person uses as their SAFE login if they have a SAFE account, or the one that they would prefer to use when they sign up for the SAFE if they don't yet have an account. To find this out, you will need to get in touch with the person in question. If you accidentally use an email address for them which they do not use in the SAFE, please just repeat the invitation with the correct email address. Invitations expire after 20 days

anyway so there is no need to delete the incorrect invitation. If an invitation is received by someone without a SAFE account, they will receive a link to accept the invitation. However, this link will only work after that person registers in the SAFE.

In line with eligibility criteria, PIs must be employees of an eligible organisation and must be resident in the UK. More information can be found here:

https://www.ukri.org/apply-for-funding/how-to-apply/check-if-you-are-eligible-for-research-and-innovation-funding/

Individuals may be named as a Co-I on more than one proposal. However, individuals may only be named as PI on one proposal for any given call.

After accepting the invitation to join the project, **all** project members should provide a description of what they will bring to the project in the "Contribution and Background" section. This should include a short track record of (as appropriate): previous involvement in technical projects, expertise with the code or scientific area, experience of managing similar projects, etc. Please ensure that for each project member this description contains enough detail to explain why that person will join the project and what that person's specific role will be. **In addition, technical staff should submit a CV** (see next section). A CV is not compulsory for PIs and Co-Is (unless they will be carrying out technical work within the project) and neither a CV nor any description of role is needed for project members who are not PIs, Co-Is or technical staff (e.g. for people who just have the role of Contact or Member). This section is to ensure the whole team have the appropriate skills, expertise and experience to carry out a successful project. This is important for all projects, but in particular where a technical staff member is less experienced, this is where relevant support for the staff member can be demonstrated within the team as a whole. The section should concentrate on any relevant software development, software engineering and management skills, as appropriate, rather than be based only on the general scientific background of the team. Things each team member may want to include are:

- A short summary of the outcomes of recent work in related projects/research.
- Your specific experience including any familiarity with the specific code(s) involved in the project.
- Previous relevant work / collaborations with other beneficiaries.
- Any experience of similar projects or other relevant experience. When referring to any previous eCSE project work, references to any final reports or associated papers should be given.
- Any training needed and where this is likely to come from.

This section has a limit of 250 words for each team member and text can be added by the team member him/herself (or anyone who can edit the proposal) once the person in question has accepted the invitation to join the proposal. The text and CVs can be added by going to the person in the relevant section (e.g. "Co-Investigators" or "Proposed Technical Staff Details") and clicking "edit".

Proposed Technical Staff Details

Please provide details of all the proposed technical staff. If there is more than one, each staff member should be added separately.

The ARCHER2 CSE team can provide technical effort for projects utilising the ARCHER2 GPU system and for projects on other systems relevant to the team's technical skills. If you wish to explore this option please contact the ARCHER2 service desk before you submit your proposal.

Consideration of the skills of the technical staff are an integral part of the review process so we encourage PIs to name and invite technical staff to the proposal. In the case that the proposed technical staff cannot be confirmed before the application submission, please use the "Add Generic Technical Staff" form and list the appropriate skills required for the candidate(s) to carry out the proposed project within section 5 (Project Overview, Technical Information and Workplan) of the proposal form. If technical staff are unnamed and not members of the ARCHER2 CSE team, please also explain in that section what plans there are for recruitment if this member of staff is not in place. Unless the member of staff is an existing member of the ARCHER2 CSE team, you will need to arrange employment at the PI's or a third-party institution. Where one or more of the proposed technical staff is/are employed by a different institution from the PI, the PI should arrange the transfer of relevant costs to the relevant institution(s).

The eCSE programme exists to enhance the UK skills base. During the course of an eCSE project we therefore expect technical staff to be employed at a UK institution (costed using the FEC model – see below). **If your situation varies from this please get in touch with the ARCHER2 service desk to discuss this in advance of your submission.**

The eCSE programme recognises that technical staff may develop skills while carrying out the project and we are very keen to encourage software developers at the early stage of their careers. The panel will assess the project's ability to deliver the planned work. This will include an assessment of the technical staff members' existing skills, any planned training to develop skills and the support on offer to them from the wider project team (e.g. PIs and Co-Is). This should all be explained in the "Background and contribution" section which should be completed by every project team member.

For each of the proposed technical staff, please provide a number for the technical effort level in person months (PMs), e.g. 6 PMs. In the case where the project includes some effort to be undertaken by the ARCHER2 CSE team, please include an entry for this effort and click the "EPCC Staff member" button when doing so.

For this call projects can request between 1 and 36 PMs of effort in total with a maximum duration of 2 calendar years.

Each member of technical staff should upload their CV along with a track record summary. Note that after you first invite technical staff to join your proposal you will not be able to edit their details or add a CV until they accept the invitation to join.

- Costing information

Please provide the total 100% Full Economic Costing (FEC) for each named member of technical staff in the proposal. The system will then work out the 80% FEC which is what would be paid should the project be funded. The costing should include direct and indirect costs. However, this should not include costs for travel, which should be given separately in the travel section. PI and Co-I salary costs are not eligible within the eCSE programme and should not be included. **Please ensure that the figure given in the SAFE form is the total 100% FEC figure and not just the salary costs.** The figure here should include all the eligible direct and indirect costs and should match the total cost given in any supplied costing document. As noted above, after you first invite technical staff to join your proposal you will not be able to edit their details (including costs) until they accept the invitation to join.

You should carry out a costing within your university using the same process you would use for a UKRI research grant and provide us with this costing. Most institutions can provide a breakdown of costs using Worktribe or an equivalent tool. This should be attached as a PDF when you submit your proposal. If the project has multiple technical staff and the technical staff are from more than one institution, please provide separate costings for each institution. Please note, for successful applications, the fee payable to individual researchers in the project team is 80% of FEC. We strongly advise you to identify staff before the proposal is submitted where possible.

We anticipate the majority of eCSE proposals will be costed using the standard FEC model. For the small number of proposals that aren't appropriate for FEC (e.g. if a freelance consultant will be providing a service) then you should provide a fully inclusive costing which should contain all possible costs including, if applicable, VAT. In such situations please get in touch in advance to discuss how to provide this.

All proposals will undergo a value for money assessment against other proposals received.

Please provide details of any existing funding for the proposed technical staff where the staff will work on projects that will overlap with the eCSE work. E.g. for a postdoctoral researcher, please list the funding organisation, funding length, start- and end-date, etc. Please indicate the level of effort that will be required to carry out that work alongside any eCSE work.

Project Schedule

- Proposed start date

Please indicate the proposed start date for the project. Successful eCSE projects are expected to start between 2-6 months after a call closes.

- Proposed duration (in months)

Please indicate the overall duration of the project in months. The maximum project duration is 2 calendar years. When considering the rate of work, technical staff are expected to focus enough of their time to the project to ensure that it will be completed efficiently and that any resulting software will be released in a timely manner to maximise the benefit to the UK HPC and AI community.

Proposal Code(s)

- Primary code(s):

Please list the main application codes involved in the project. These codes should be described in more detail in the proposal document. There is a set of questions related to the codes:

- Existing funding for code(s) (max 200 words):

It is important that the Panel understand how the work to be carried out in the eCSE project differs from that funded by other sources for the code(s) in question. Please provide a clear and concise summary of any existing funding and how that differs or overlaps with the work planned for the eCSE project.

- Approximate current number of users of the code(s) in the UK:

- Explanation of the number of UK users:

- Approximate current number of users of the code(s) world-wide:

- Explanation of the approximate number of global users:

- Percentage of UK code(s) users expected to benefit from this project:

- Explanation of how you arrived at the percentage of UK users expected to benefit from this work:

- Percentage of non-UK code(s) users expected to benefit from this project:

- Explanation of how you arrived at the percentage of of non-UK users who will benefit from this work:

It is essential that the eCSE programme can demonstrate an overall benefit to the UK research community. The above questions are about usage of the code within the UK and the overall global usage and the expected benefit of the improvements of the code. Please answer these questions as accurately as you can. In the case where these figures are estimated, please explain how the estimate was reached.

If your project involves multiple codes then please provide figures for all the codes combined (if the improvements benefit all the codes) or if, for example, the project involves the interfacing of two codes, please provide figures for the two codes in use together. If you have any questions about this, please contact the service desk.

- Travel plan
- Travel Cost Estimate (in Pounds)

The eCSE programme funds reasonable travel for collaboration meetings and funds one national or international trip for each technical member of staff. Travel for other activities is not suitable for the eCSE.

Collaboration Meetings

During the lifetime of an eCSE project, we will fund reasonable travel expenses for collaboration meetings between partners.

This covers travel - within the UK only - for members of an eCSE project team to meetings with other project team partners, and to appropriate meetings required to carry out the eCSE project. Travel to or from destinations outside of the UK will not be funded, nor will travel to attend workshops or conferences, or to visit users/developers of a code outside of the project.

The funding which can be requested in this proposal can be used to fund travel to meet with colleagues on the same project, e.g. PIs, Co-Is or named technical staff. As a guide, for every 4 person months of effort awarded, we would expect approximately 1 single-day visit for any individual project team member. For example, for a project with 12 person months of effort awarded, this may be one 3-day meeting with a single person travelling to this meeting, or may be one single day meeting with 3 people travelling across the whole project.

Conferences/workshops

In addition to this, travel funds may be requested to send each technical member of staff to one national or international conference or workshop to help disseminate their work on the project.

Breakdown of Costs

Please briefly list the travel plan, e.g. travel purpose, destination, etc. with a breakdown of the costs. An estimate of the overall travel cost should be provided as well. In the case where there is more than one member travelling, please further break down the cost per person.

IV.Project Proposal

All files attached to the proposal in the SAFE must be submitted in PDF format: Please ensure that all documents are submitted as PDFs and that any PDF documents uploaded are not locked in such a way that prohibits either copying information from them or combining them into larger documents.

The project proposal for eCSE calls should consist of the following 7 sections. The guidance for the limits for each section is given below.

Please observe the page limits. Each section should contain enough information for a reviewer to understand what the aims of the project are together with the underlying context and technical detail. However, it is not necessary to use all of the space available, especially for shorter projects.

1. Project Title

Please use the same project title here that you use in the SAFE form

2. PI Name and Institution

Enter the name of the PI of the eCSE proposal and the institution of the PI

3. Description of code(s)

maximum of 2 page

This section should be used to describe the code that will be worked on during the project and should include

- An overview of the code, for example
    - A short description of what the code is and what it does
    - The complexity the code – e.g. in terms of size/structure/etc.
    - Programming languages used in the code
- Any underlying dependencies, for example
    - Specific compilers, libraries or dependence on other software
- Links where appropriate
- Current status of the code, for example
    - What platforms has the code been run on?
    - Which communities utilise the code to deliver their research
    - If the code is associated with any ARCHER2 consortia (https://www.archer2.ac.uk/research/consortia/), please state which consortia
    - Scaling or performance data
        - This could be performance data from profiling, comparison with CPU for a GPU code, or scaling with no. GPUs for multi-GPU codes

4. Project Objectives and success metrics

maximum of 1 page

Please state the intended objectives of your project. The assessment process will prioritise funding projects with objectives that complement, support and enable research in the existing portfolios, or the strategic priorities for the councils and their associated communities. In addition to forming part of the proposal assessment criteria, should your proposal be accepted you will be asked to report against these objectives, and this will be used to assess the final success of your project

As a guide we would expect 1-2 objectives for a proposal requesting <6 PMs of effort and around 5-6 objectives for a proposal with the maximum requested effort of 36 PMs.

Examples of objectives include but are not limited to:

- Transforming existing software that targets CPU architectures into software that can exploit GPU-based architectures (in part or in full)
- Implementation of algorithmic improvements within existing GPU software
- Improving the portability of GPU software (e.g. converting CUDA-based software to run on a wider range of architectures)
- Improving the performance of software running on GPU-based architectures
- Improving the scalability of software to enable effective use of an increased number of GPUs
    - E.g. making software that can run on a single GPU able to exploit multiple GPUs in parallel or making single-node, multi-GPU software scale better across multiple nodes with GPUs
- Improving GPU-based software to enhance sustainability and maintainability
- Improvements to GPU-based software to allow new research to be carried out
- Adding new functionalities to existing GPU-based software or enhancing existing GPU software for use in new research areas/workflows

For each objective, applicants should provide an associated set of success metrics, **metrics that are specific and measurable** and can be used to assess whether the objective has been met at the end of the project.

Note that eCSE funding cannot be used for scientific research itself or for the development of new algorithms.

Applicants are encouraged to list their objectives and success metrics, for example as a table or bulleted list.

5. Project Overview, Technical Information and Workplan

maximum of 2 pages

This section should give a general description of the proposed project. This section should also provide the technical background for the proposed project and demonstrate a good knowledge and understanding of previous and current work in the related area. The technical information provided may include, but is not limited to:
- The major algorithms and functional updates related to the code to be used in the proposed project.
- The important prerequisites for the proposed project, e.g. the key algorithms, libraries, software to be installed, etc.
- If there are multiple codes available which have similar functionality to the code you are proposing to work on, please justify your choice of code.

This section should also include a Gantt chart (or equivalent) of the workplan of the proposed project, including the implementation plan of the technical work within the given time schedule, the specific milestones to be completed and the personnel efforts

required for the eCSE project (in person months).

Any potential risks should be identified and stated clearly together with their likelihood of occurring and any possible solutions.

Projects may utilise the GPU component of ARCHER2 or other suitable GPU resources to complete the technical work. If the proposal plans to use the GPU component of ARCHER2, successful projects will be given access to these resources. If projects plan to utilise other systems, you should ensure you have suitable resources available to complete the project successfully. Please contact and arrange this access with the relevant service provider before submission. Please explain in this section on which system(s) the technical work will be carried out (e.g. ARCHER2 GPU development system or elsewhere - if elsewhere please give a brief summary and links as appropriate).

6. Sustainability, maintenance, validation and availability of code(s)

maximum of 1 page

This section should include information on how the code(s) will be made available to users, how the code(s) will be maintained, what coding standards will be used, etc. This section should also describe the availability of the code(s) on completion of the project, both for users wishing to run the code(s) and users wanting access to the underlying source code(s). This should include any information on the licensing model.

7. Impact and Benefits

maximum 1 page

Applicants should describe the potential impact of the science enabled by this work. Any scientific advancements which will be facilitated/enabled by the completion of the proposed project are expected to be included in this section. This section should also describe how the applicants plan to achieve this impact (likely after the end of the project) and the anticipated timescales.

Please note that the assessment criteria for all eCSE proposals is the same and all are expected to provide impact and benefits to the UK HPC and AI community. Applicants should identify and describe both the computational and scientific benefits considering the following aspects:

- Why the proposed project is needed and what outcomes/benefits are to be expected.
- Who will be the beneficiaries for this proposed project (the applicants' own research, other research groups, science/computational communities, other disciplines, etc.) and how will the achievement impact the beneficiaries.
- The section should also explain how the outcome(s) of the proposed project will benefit the UK HPC and AI user community explicitly.
- Explain how the proposed work complements, supports and enables research

in the existing UKRI portfolio and the strategic priorities of the councils.

V. Supporting Documents

Various documents should be included with your proposal as PDFs:

- **Proposal Document:** Your submission must include a completed Proposal Document
- **CVs**: CVs of each technical staff member should be added within the "Proposed Technical Staff Details" section.
- **Costing documents**: For each named technical staff member, who is not part of the ARCHER2 CSE team, costings should be provided within the "Proposed Technical Staff Details" section together with supporting costing document(s) (see above). Please provide at least one document per institution. Staff costings within one institution may be combined into one document and if this is the case, that one document should be added to one of the staff members covered by the document and there is no need to add the same document multiple times within the form.
- **Letters of support**: Supporting letters from UK research groups which give details of the scientific justification, or from code maintainers supporting improvements to their codes, are also encouraged. These should be uploaded in the "Supporting Files" section near the bottom of the on-line form.

VI. Evaluation Process and Notification of Decisions

Applicants will receive an acknowledgement of submission when a proposal has been received by the eCSE team.

Each application is reviewed by the eCSE Review Panel who will rank each of the proposals and make decisions on which projects to award funding to. The panel will be made up of experts in the scientific and technical areas. The panel will consider the proposal, and recommend funding it in full, funding it at a reduced effort level, or rejecting the proposal.

At the end of the eCSE Panel Review process, the Panel decisions will be sent to applicants along with any comments made by the panel. The Panel's decisions are final.

The applications will be reviewed based on the following assessment criteria:

Project team Applicants

The proposal should provide track records of the proposed team members who will carry out the work in the proposed project, and demonstrate that they are able to deliver a successful project.

Project Objectives and success metrics

Clear and concise objectives with appropriate success metrics (quantifiable where appropriate) should be provided. The number of objectives and success metrics should be appropriate for length of the project. The extent to which the objectives complement, support and enable research in the existing UKRI portfolios, or the strategic priorities for the councils and their associated communities (reviewers may also wish to refer to Impact and Benefits section of the application form) should be clear within the proposal.

Project Overview, Technical Information and Workplan

The proposal should include sufficient technical information to provide confidence that the proposed project will be successfully delivered with an appropriate plan for the technical work, management and required resources.

Impact and Benefits

The proposal should explain why the proposed project is needed and what the expected computational and scientific benefits will be, as well as the specific benefits to the UK HPC and AI community. The proposal should identify and describe the impact activities to be undertaken to ensure the project's potential benefits are achieved. Please also consider the sustainability of the software beyond the end of the project.

The final decisions of the eCSE Review Panel will be sent to applicants including the feedback provided by the Panel. Each successful proposal will be provided with a named contact within the CSE team. All unsuccessful applicants will be provided with constructive feedback.

VII. *Further Information and Assistance from ARCHER2 service desk*

Please see the eCSE page for the general information about the eCSE call and support. If you have any queries or require assistance regarding the eCSE application, please contact the ARCHER2 service desk: support@archer2.ac.uk.