

# Computational Science and Engineering: Software for the Future II

**Call type: Invitation for proposals**

**Call opens: 26<sup>th</sup> March 2014**

**Intent to submit deadline: 28<sup>th</sup> April 2014 16:00**

**Closing date for full proposals: 28<sup>th</sup> May 2014 16:00**

**Related Themes: Research Infrastructure, ICT, Physical Sciences, Engineering, Maths**

## Summary

In both the recently published EPSRC E-infrastructure roadmap and the EPSRC Software as an Infrastructure strategy, the importance of software development and the need to invest in people and training in this area has been strongly highlighted. EPSRC has therefore made a long-term commitment to support software development, ensuring that funding continues to support leading scientific research and key codes used by the Engineering and Physical Sciences community.

Subject to quality, up to £4M of funding is available for projects focused on the development of software that is used in computational science and engineering. **All proposals submitted to this call must fall within the EPSRC remit.**

As part of an on-going series of regular software development calls, this call covers the development of novel code, the development of new functionality for existing codes, and the development and re-engineering of existing codes. Strategic drivers are: developing code for emerging hardware architectures; developing researchers with key software engineering skills and software sustainability.

In order to allow maximum time for the selection of appropriate reviewers and panel members all applicants **must** register their **intent to submit** using the electronic 'Intent to submit' form on the Software for the Future II call page on the EPSRC website. The form **must** be submitted to EPSRC by **16:00 on Monday 28<sup>th</sup> April 2014**. Full applications will **not** be accepted where EPSRC has not received an intent to submit form.

**Collaborative Computational Projects (CCP):** As part of this call, EPSRC would like to invite the existing portfolio of CCPs ([www.ccp.ac.uk](http://www.ccp.ac.uk)) to submit new, innovative and challenging software development **Flagship projects**. CCP Flagship Projects should be aimed at serving the research community that the CCP represents. **All Flagship projects submitted to this call must underpin research that falls within the EPSRC remit.**

## Background

Software developed for experimental facilities and instrumentation, modeling, simulation and data-analysis is a critical and valuable resource. Software and algorithm development represents major investments in skilled scientists and engineers and the large suite of codes and algorithms used in research should be regarded as a research infrastructure, requiring support and maintenance along the innovation chain, and throughout its lifecycle.

Through the publication of the **EPSRC E-infrastructure roadmap** and the **EPSRC Software as an Infrastructure strategy**, EPSRC has recognised the importance of investing in software development and ensuring that funding continues to be used to support leading scientific research and key codes used by the EPS community as well as skills, training and career development for researchers in this field.

Over the last five years EPSRC has invested approximately £9M per annum in computational science and engineering software covering a range of activities from new algorithm development at the leading edge of research applications, through software development, to code maintenance.

This funding opportunity forms part of an on-going series of software development calls, with a further call planned for 2015/16.

For more information on the EPSRC E-infrastructure roadmap and the EPSRC Software as an Infrastructure strategy, please see the EPSRC website:

EPSRC E-infrastructure roadmap:

<http://www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/strategy/roadmap/Pages/roadmap.aspx>

EPSRC Software as an Infrastructure strategy:

<http://www.epsrc.ac.uk/SiteCollectionDocuments/other/SoftwareAsAnInfrastructure.pdf>

## Aims and Scope

The focus of this call is on the software that is used in computational science and engineering. This covers:

- The development of novel code in new or existing application areas to enable new research to be carried out.
- The addition of new functionality to existing codes to address new research challenges.
- The development and re-engineering of existing codes for emerging hardware architectures.

**Proposals where the software development addresses application areas that are outside of the EPSRC remit will not be considered.**

Strategic drivers for this call are:

- **Developing code for emerging hardware architectures:** This includes co-design, taking into account the direction hardware is going, preparing for potential new architectures, making the code platform-agnostic, and addressing energy efficiency issues in the software.
- **Developing of researchers with key software engineering skills:** A focus on the acquisition of skills in software engineering by the research staff involved in the projects, providing short term funding for early career researchers to immerse themselves in different research environments (e.g. maths, computer sciences and application areas) through discipline hopping type activities and participation in short training courses outside their domain. This also includes promoting international and industrial collaboration through secondments and people exchange.
- **Software sustainability:** Ensuring best practice in software development (for instance, the use of code repositories, development of documentation, and understanding of user requirements) is embedded in projects from the beginning, to enable reusable and reliable software. This includes supporting and encouraging the development of software management plans and where appropriate embedding professional software developers / research software engineers in to project teams from the start.

## Funding available

Up to £4M is available for this call and EPSRC expect to fund between 5-7 projects. The **research enabled** by the software development projects must be novel and cutting edge and **must be within the EPSRC's remit**. Software development projects submitted to this call should be **no longer than 3 years in duration**.

Interdisciplinary proposals will be viewed favourably. For example, proposals may involve computational scientists and engineers from a range of application areas working together; alternatively these projects may throw up novel research questions in computer science and mathematics, and applicants are encouraged to work with colleagues from these fields in developing their proposals. Attention is drawn in particular to the ICT Theme's priority in **Many-core architectures and concurrency in distributed and embedded systems:**

<http://www.epsrc.ac.uk/research/ourportfolio/themes/ict/introduction/manycore/Pages/manycore.aspx> .

Building links with international colleagues is welcomed and collaboration with industry (either software companies or software users) is also encouraged. Applicants can include requests for funds to enable these activities.

Where appropriate, the costs of training courses for researchers within the project team can be included in the proposal.

Applicants to this call can apply for time on or the cost of using the national HPC service, regional/university machines, or the Hartree Centre machines. Further details are given in **Appendix 1**.

The project teams for all proposals submitted to this call must include the necessary skills and experience to ensure high quality software development. If this expertise is not available within the research group or locally, the involvement of expert software developers from elsewhere is encouraged, and any associated costs can be included in the application. Further details are given in **Appendix 2**.

**Collaborative Computational Project Flagship Projects:** As part of this software development call, EPSRC would like to invite the existing portfolio of CCPs ([www.ccp.ac.uk](http://www.ccp.ac.uk)) to submit new, innovative and challenging software development **Flagship projects**. Flagship projects can be submitted by individual CCPs or collaboratively by more than one CCP. CCP Flagship projects should be community driven projects, strongly aligned with the interests and strategic requirements of the research community that the CCP represents. **All** Flagship projects submitted to this call **must underpin research that falls within the EPSRC remit**. Flagship projects **should be no longer than 3 years in duration**. Further information on the future funding model for CCPs is available in **Appendix 3**.

## Equipment

Where possible, researchers are asked to make use of existing facilities and equipment, including those hosted at other universities.

No single items of equipment costing over £10,000 (inc. VAT) in total will be supported as part of this call. Equipment under £10,000 should be applied for under Other Directly Incurred costs as usual.

## Eligibility

Applicants are allowed to submit **one** software development proposal as Principal Investigator to this call.

Each CCP is allowed to submit **one** Flagship project.

For information on the eligibility of organisations and individuals to receive EPSRC funding, see the EPSRC Funding Guide:

<http://www.epsrc.ac.uk/funding/guidance/fundingguide/>

As this call is a targeted funding opportunity provided by EPSRC, higher education institutions, and some research council institutes and independent research organisations are eligible to apply. A list of eligible organisations to apply to EPSRC is provided at: <http://www.rcuk.ac.uk/funding/eligibilityforrcs/>

## How to apply

### Submitting application

#### Intent to Submit

In order to anticipate demand and allow maximum time for the selection of appropriate reviewers and panel members, all applicants **must** register their intent to submit using the electronic 'Intent to submit' form on the Software for the Future II call page on the EPSRC website:

<http://www.epsrc.ac.uk/funding/calls/2014/Pages/softwarefuture.aspx>

The form must be completed by **16:00 on Monday 28<sup>th</sup> April 2014**.

The intent to submit should contain the following information:

- Suggested title for the project.
  - For CCP Flagship projects the title should be in the following format,  
**CCP Flagship: Suggested title for the project.**
- Name, institution and e-mail address of the proposed Principle Investigator.
- A list of other potential Co-investigators and their institutions.
- A one-paragraph summary of the potential research proposal.
- A numbered list of objectives for the project.

If an intent to submit is **not** received a full proposal will not be accepted. In the event of multiple submissions from the same institution or group EPSRC reserve the right to require bids to be consolidated prior to final submission.

### **Full Proposals**

You should prepare and submit your proposal using the Research Councils' 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 for the Future Call II' call.

For collaborative, multi-institutional projects, applicants are encouraged to submit their application on a single Je-S form.

For **CCP Flagship Projects** the title must be in the following format, CCP Flagship: Title.

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 Wednesday 28<sup>th</sup> May 2014.**

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 (<http://www.epsrc.ac.uk/funding/guidance/>) which should be consulted when preparing all proposals.

### **Guidance on writing application**

For general advice on writing proposals see:  
<http://www.epsrc.ac.uk/funding/guidance/preparing/>

If the attachments are uploaded as Word documents, please be aware that once the application has been submitted to the Council/Funder, all the attachments

will be converted and held as an Adobe Acrobat file (PDF). Also please note, that whilst we support a wide range, **we do not support all MS Word font types**. Therefore if an unsupported font type is used a different font type may be substituted which may result in changes to the layout of the document. For this reason we recommend that the documents are converted to PDF files before uploading.

The full proposal should consist of the following completed documents. Where appropriate, call specific advice is given. Applicants are advised to consider the assessment criteria and strategic drivers of the call, and to ensure that they address these in their application:

### **Case for support (up to 8 sides of A4)**

- **Track Record (up to two sides of A4):** The proposed project team should submit a tailored track record which highlights their skills, expertise and experience in software development.
- **Description of proposed research and its context (up to six sides of A4):** As well as providing details of national importance, proposal objectives and programme and methodology, the case for support should demonstrate a knowledge and understanding of the past and current work in the subject area in the UK and internationally. The applicants should also explain how the proposed project meets the aims and strategic drivers of this call.

### **Pathways to impact document (up to two sides of A4)**

- <http://www.rcuk.ac.uk/ke/impacts/>
- A specific section of the pathways to impact document should be dedicated to detailing the software management plan for the proposal. This should include information on what software outputs (including documentation and other related material) will be produced, who is responsible for releasing the software, the revision control process to be used, and the licensing for each output. For further guidance and information on what to consider in the software management plan please see: <http://www.software.ac.uk/resources/guides/software-management-plans>

### **Justification of the resources requested (up to two sides of A4)**

#### **Work plan (up to one side of A4)**

#### **CVs (up to two sides of A4 each)**

- For named post-doctoral researchers, visiting researchers and researcher co-investigators, where applicable. No CVs will be accepted for PI and Co-Is.

#### **Statements of support from any project partners (no page limit)**

- Letters of support from all project partners should be included as an attachment.

#### **Letters of support**

- Letters of support should **only** be submitted where there is a direct and clear commitment to a specific aspect of the proposals from an organisation that cannot be listed as a project partner.

- For example, if software development support is being requested, proposals should include a letter of support from the organisation or individual providing the software development expertise, committing to participate in the project should the proposal be successful.

### **Technical assessment (no page limit)**

- Any proposals requesting ARCHER time **must** have a technical assessment attached. Please note these can take up to 10 working days to complete.

Additional documentation will not be accepted after the deadline. Please note that proposals not accompanied by the correct documentation will be rejected.

### **Specific guidance for CCP Flagship projects**

Due to the community driven nature of the CCP Flagship projects, there are a number of additional aspects the CCPs will be expected to cover in their case for support and pathways to impact document:

#### **Cover Letter**

- A cover letter must be submitted with all CCP Flagship projects. The cover letter should outline which CCP/s have been involved in the formulation of the project and provide confirmation that the submission of the Flagship project has been agreed by the CCP chair and working group.

#### **Case for Support**

- **Track Record:** The track record should demonstrate how the proposed Flagship project builds on the CCPs track record and work with the community and how it complements the existing projects and funding that the CCP receives.
- **Description of proposed work and its context:** The case for support should demonstrate how the proposed flagship project strongly aligns with the interests and strategic requirements of the research community that the CCP represents. The case for support should also outline how members of the CCP community will be involved as the project develops.

#### **Pathways to impact document**

- A section of the pathways to impact document should be used to highlight the groups within the broader CCP community that will have an interest in the progress and the outputs of the Flagship project and how they will be engaged during the course of the project.

## **Assessment**

### **Assessment process**

Proposals will be sent to external peer reviewers for their comments. Where sufficiently supportive reviewer comments have been received, Principle Investigators will be invited to submit a response to the reviewers' comments. Proposals will then be considered and prioritised for funding by a peer review panel.

Applicants should note that peer reviewers and panel members will be drawn from a pool which will include software development experts, computational

scientists and engineers, computer scientists and mathematicians. EPSRC reserve the right to sift proposals at any stage to ensure all proposals fit the call.

**CCP Flagship Projects:** Due to the community driven nature of the CCP Flagship projects, the **CCP Flagship projects will be prioritised on a separate list to the software development proposals during the peer review panel.** The prioritised list of CCP Flagship projects will then be tensioned against the software development proposals prior to a funding decision being made.

## Assessment criteria

The proposals will be assessed against the following criteria:

- Fit to the scope of the call and how the proposal addresses the strategic drivers.
  - **CCP Flagship Projects:** Alignment to community requirements.
- Quality, including novelty of the research enabled, quality of the software engineering proposed, the appropriateness of the proposed methodology.
- Importance, including contribution to EPSRC's strategic priorities.
- Quality of the proposed pathways to impact, including the quality of the software management plan, and of the plans for collaboration.
- Relevant experience and knowledge of applicants, including the balance of the skills within the project team.
- Resources and Management.

## Guidance for reviewers

Information about the EPSRC peer review process and guidance for reviewers can be found at: <http://www.epsrc.ac.uk/funding/peerrev/review/>

## Key dates

Activity	Date
Call opens in Je-S	26 <sup>th</sup> March 2014
Intent to submit deadline	16:00, 28 <sup>th</sup> April 2014
Call closes in Je-S	16:00, 28 <sup>th</sup> May 2014
Principle Investigator responses	Early August 2014
Panel meeting	September 2014

## Contacts

Requests for help and advice concerning the writing and costing of your proposal should be addressed to your institutional Research Office in the first instance.

If you have any questions about preparing and submitting your proposal using Je-S, please contact the Je-S helpdesk ([JeSHelp@rcuk.ac.uk](mailto:JeSHelp@rcuk.ac.uk), 01793 444164).



For other queries not addressed in the call document please contact:

**Dr Louise Tillman**

Senior Portfolio Manager, Research Infrastructure  
Telephone: 01793 44 4073

**Dr Daniel Emmerson**

Portfolio Manager, Research Infrastructure  
Telephone: 01793 44 4112

**Or via e-mail at:** [EPSRCsoftware@epsrc.ac.uk](mailto:EPSRCsoftware@epsrc.ac.uk)

For access to necessary computing resources, see **Appendix 2**.

For software development support, see **Appendix 3**.

### **Change log**

<b>Name</b>	<b>Date</b>	<b>Version</b>	<b>Change</b>
Louise Tillman	March 2014	1	N/A

## Appendix 1: Access to Computing Resources

Applicants should include the necessary computing resources needed for the project.

For access to the **national HPC service, ARCHER**, please follow the process described on the web:

<http://www.epsrc.ac.uk/research/facilities/hpc/access/Pages/apply.aspx>

For help and advice, please contact the Help Desk on [support@archer.ac.uk](mailto:support@archer.ac.uk). Please note that a technical assessment will need to be attached to the proposal on submission.

Following recent capital investments from UK government the Department has established **the Hartree Centre** in collaboration with IBM. This outward-facing centre offers a range of services including collaborative software development and access to a range of novel hardware platforms (98304 core Blue Gene/Q, Blue Gene Active Storage, iDataPlex, NextScale, ARM, nVidia Tesla GPU, Intel Phi and Maxeler MPX-X).

For access to the Hartree Centre machines, please contact: Michael Gleaves, Head of Business Development, The Hartree Centre, STFC Daresbury Laboratory e-mail: [Michael.Gleaves@stfc.ac.uk](mailto:Michael.Gleaves@stfc.ac.uk), tel: 01925 603710  
<http://www.stfc.ac.uk/hartree/default.aspx>

For access to your **local or regional machines**, please contact the relevant person at your institution or the regional centres directly. It is permissible to include the cost of this access on the grant.

EPSRC supported regional centres:

<http://www.epsrc.ac.uk/research/ourportfolio/themes/researchinfrastructure/subthemes/einfrastructure/hpc/Pages/computingcentres.aspx>

HPC Wales: <http://hpcwales.co.uk/services> or e-mail direct to [info@hpcwales.co.uk](mailto:info@hpcwales.co.uk) for further access information.

## Appendix 2: Access to Software Engineering Support

Applicants may have access to local expertise that can provide the support needed. However, the following organisations also offer support, and can be approached during the development of proposals. If software development support is being requested, proposals **must** include a letter of support from the organisation or individual providing the software development expertise, committing to participate in the project should the proposal be successful.

**Edinburgh Parallel Computing Centre** Founded at The University of Edinburgh in 1990, EPCC is a leading European centre of expertise in advanced HPC research, technology transfer and the provision of supercomputer services. It has a portfolio of successful and high-impact software engineering projects collaborating with academic research groups from the UK and beyond. The centre has 20 years of experience of scientific computing, including both application development and fundamental HPC research, delivered by an expert team of researchers, software programmers and project managers. The centre's activities involve computing platforms as diverse as multi-core desktop computers; novel technologies such as GPGPU, Xeon Phi, ARM and FPGAs; big data facilities; and capability-scale national services. EPCC manages the current national service system, ARCHER, and provides the Computational Science and Engineering support for the service.

Contact: Dr Andrew Turner, EPCC Applications Group, University of Edinburgh  
e-mail: [a.turner@epcc.ed.ac.uk](mailto:a.turner@epcc.ed.ac.uk), tel: 0131 650 5845 <http://www.epcc.ed.ac.uk/>

**NAG Ltd** The Numerical Algorithms Group (NAG) has over 40 years experience of taking software developed in academia, transforming it into high-quality code, and delivering it to users via commercial products. In 2009 NAG provided training in "Best Practice in HPC Software Development" for EPSRC grant holders. NAG offers expertise in programming for portability, designing and implementing test and benchmarking suites, source code maintenance and documentation production.

Contact: Dr Mike Dewar e-mail: [Mike.Dewar@nag.co.uk](mailto:Mike.Dewar@nag.co.uk), tel: 01865 518055  
[www.nag.co.uk](http://www.nag.co.uk)

**Software Sustainability Institute** The Software Sustainability Institute is the UK's national facility for cultivating world-class research with software. The Institute provides advice and expertise on best practice for developing reproducible, reusable and reliable software; the role and recruitment of software developers within an academic software team; meeting the software training needs of a research project; and developing a sustainable user and developer community. The Institute also provides online guides and software evaluation tools, and has a team of experts who work with research projects to develop and/or review software. It is the UK Coordinator for the Software Carpentry training initiative. The Institute will consider partnering with projects that wish to improve the sustainability of new and existing software.

Contact: Neil Chue Hong e-mail: [info@software.ac.uk](mailto:info@software.ac.uk), tel: 0131 650 5957  
[www.software.ac.uk](http://www.software.ac.uk)

**STFC** STFC's Scientific Computing Department has over thirty years' experience in the design, implementation and development of world leading scientific

software. It is internationally recognised as a Centre for parallelisation, optimisation and porting of existing software to leading edge and novel architecture systems. In addition to domain expertise in a wide range of disciplines the Department also has strong software engineering and numerical algorithms expertise. Following recent capital investments from UK government the Department has established the Hartree Centre in collaboration with IBM. This outward-facing centre offers a range of services including collaborative software development and access to a range of novel hardware platforms (98304 core Blue Gene/Q, Blue Gene Active Storage, iDataPlex, NextScale, ARM, nVidia Tesla GPU, Intel Phi and Maxeler MPX-X).

Contact: Michael Gleaves, Head of Business Development, The Hartree Centre, STFC Daresbury Laboratory e-mail: [Michael.Gleaves@stfc.ac.uk](mailto:Michael.Gleaves@stfc.ac.uk) tel: 01925 603710.

## Appendix 3: Collaborative Computational Project Funding Model

### Background

Collaborative Computational Projects (CCPs) bring together the major UK groups in a given field of computational research to tackle large-scale scientific software development projects, maintenance, distribution, training and user support. There are hundreds of UK groups participating in the CCPs and extensive collaborations with international groups and industry.

CCPs currently include support for the following activities:

- Core support provided through a Service Level Agreement with STFC's Daresbury Laboratory.
- Networking activities.
- Flagship software development projects.

A full list of CCPs can be found here: <http://www.ccp.ac.uk/>.

In 2010 EPSRC held a call for Statements of Need for CCPs to assess which research areas were of the highest priority to include within the EPSRC supported CCP portfolio. In 2011, following the prioritisation of the Statements of Need and a call for full proposals, EPSRC awarded funding to 8 CCPs:

- **ASEArch:** Algorithms and Software for Emerging Architectures
- **CCP-BioSim:** Bio molecular simulation at the life sciences interface
- **CCP5:** The computer Simulation of Condensed Phases
- **CCP12:** High Performance Computing in Engineering
- **CCP-NC:** Collaborative Computer Project for NMR Crystallography
- **CCP9:** Computational Electronic Structure of Condensed Matter
- **CCPQ:** Quantum dynamics in Atomic Molecular and Optical Physics
- **CCPi:** Tomographic Imaging

As part of the joint EPSRC/NSF Software for Grand Challenges in the Chemical Sciences call in 2012 an additional CCP was supported:

- **CCP-SAS:** Collaborative Computational Project for advanced analyses of structural data in chemical biology and soft condensed matter

### Future Funding Model

Subsequent to a mid-term review of the current portfolio of EPSRC CCPs, the following changes will be made to the CCP funding model:

- **CCP Flagship Projects:** CCPs will be invited to submit new, innovative and challenging software development Flagship projects to the regular software development calls run by the Research Infrastructure team at EPSRC. This will allow the quality of the Flagship projects to be assessed through robust peer review and tensioned against other software development proposals. A further software development call is planned for 2015/16.
- **CCP Networking and Core Support:** A call for proposals will be issued in June 2014 to provide funding for the networking, training and core support

activities carried out by the CCPs. This call will be open to both existing and new CCPs within the EPSRC remit. Proposals will be considered by a peer review panel, with funding decisions to be made at the end of 2014.