Guidance Note for Applicants for Access the National High Performance Computing Services

Please note that this document is aimed at applicants whose research is in the remit of EPSRC. As access mechanisms can vary between Research Councils, applicants whose research is outside the remit of EPSRC are advised to contact the relevant Research Council for further details.

For information on the eligibility of organisations and individuals to receive EPSRC funding, see the EPSRC Funding Guide: http://www.epsrc.ac.uk/ResearchFunding/HowToApply/FundingGuide.htm.

1. National High Performance Computing Services

Two national high performance computing services are currently in operation:

- HPCx provided by a consortium led by the University of Edinburgh, partnered by CCLRC (Council for the Central Laboratory of the Research Councils) and IBM. For more details of the services offered see http://www.hpcx.ac.uk/
  This service is currently due to end on 31st January 2010

- HECToR provided by the University of Edinburgh, Cray and NAG Ltd. The HECToR hardware will be provided in three phases over the service's duration with the first phase entering service on 1st October 2007, the service is scheduled to run until October 2013. For more details of the services being offered see: http://www.hector.ac.uk/

These guidance notes provide:

- An overview of the access routes to the HPC services (section 2)
- Details of how to apply through each access mechanism (section 3)

Additional information is given on:

- The Allocation Units system for awarding computing resources (section 4)
- The consortium model (section 5)
- Software support (section 6)
- Contact details (section 7)

2. Overview of access routes to HPC facilities

There are two main classes of access to high performance computing facilities, each split into two sub classes. These are detailed below.

N.B. Class 1a access is available on both HPCx and HECToR. All other access routes are available on HECToR only; they are not available on HPCx.

Peer reviewed access to the National Services:

Two peer reviewed routes are available to the National Service:

- **Computer Resource in Support of an EPSRC Research Proposal (Class 1a on technical assessment form)**

  Under this mode of access, applicants can request compute time on a national service as part of their EPSRC Responsive Mode or Call application. Class 1a applications to use the 'service are uncapped and open for the duration of the research grant they support. Compute time allocations will be assessed along with all other fEC resources requested by the applicant. As with all other resources, allocation requests will be assessed with respect to the quality of the scientific case and need to be justified in the application's Justification of Resources. Further details on EPSRC's standard peer review process can be found at:

  http://www.epsrc.ac.uk/ResearchFunding/HowToApply/default.htm

  In the case of Calls for Proposals issued by EPSRC, compute resources will also be assessed with respect to all other resources requested. However, due to the targeted nature of Calls some restrictions or changes to the Peer Review process may be in operation, as such applicants are advised to read the call documentation thoroughly before submission.

- **Direct Access to the National Service (Class 1b on technical assessment form)**

  Within this mode of access applicants can request access to **compute time only** on the national service. Requests for compute time on the national service will, as for Class 1a applications, be uncapped; however, usage will be restricted to a period of six months from the requested start date of award. Review of proposals received will be via a Resource Allocation Panel selected from a cross section of HPC users within the Engineering and Physical Sciences community. The RAP will assess the scientific quality and level of computing resource requested as presented, there will be no postal refereeing of proposals submitted under this mechanism. Applicants should note that Direct Access represents discretionary access to the HECToR system and is not a Research Council grant. As such no fEC costs will be considered under this mode of access.

  The Resource Allocation Panel meets every 4 months. Upcoming panel dates and their corresponding closing dates can be viewed at the link below:

  http://www.epsrc.ac.uk/CallsForProposals/hectorrapcall.htm

  Applicants will be notified within 1 week of the panel meeting and must start access within one month of the panel meeting.

  Researchers should apply for class 1b access if they require access to a significant amount of computing resources (> 1,000,000 AU) on a short timescale and do not require resources other than compute time e.g. proof of concept calculations in aid of a future grant proposal, testing code improvements at scale, production runs at core counts greater than that available on locally available clusters.

Non peer–reviewed access to the national services

Non-peer reviewed access to the national services is intended to provide researchers with compute resource to investigate the potential benefits and any immediate issues regarding the running of their codes on the national service. As with peer-reviewed activity this access class is also split into two routes:

- **Pump priming activity (Class 2a on the technical assessment)**,

  Under this access route it is anticipated that most applications will be exploratory in nature, utilising the time to gain a feel of whether usage of the service is of benefit to their research. As such this activity is aimed at new-users and those transitioning from other HPC platforms. All applicants will need to complete a technical assessment form available from:

  http://www.hector.ac.uk/howcan/admin/apply/form.doc

  The technical assessment form is used to check the technical suitability of the work proposed for HECToR and is not an assessment of the underlying science, EPSRC will however review the form to check remit fit of the usage proposed. Under pump-priming activity users will be allowed access to up to 200,000 AUs of computing resource on the system for a period of six months from EPSRC approval of access to the system.

- **Access to support Distributed Computational Science and Engineering applications (Class 2b)**

  Distributed Computational Science and Engineering Support is provided by the HECToR service in order to assist current and prospective HECToR users to optimise and develop their application codes for use on the HECToR system. For details see:

  http://www.hector.ac.uk/cse/distributedcse/

  Researchers should apply through this route if they wish to apply to a DCSE call but do not have compute resource at the time of application. Applicants can request a maximum of 400,000 AU in support of their DCSE proposal. HECToR time will be released on confirmation of DCSE support from NAG. Due to the limited resource, it is envisaged that this route will be used to support short-term activities e.g. code development in order to migrate from a mid-range system to national service or to support development work prior to submitting a full proposal to peer review. Access To the compute time will be allowed for the duration of the DCSE project.

3. How to apply for access

3.1 Technical assessment

Prior to submission to the Research Councils for any access mechanism, all Principal Investigators should obtain a technical assessment of their proposal from the HPCx / HECToR service provider. This is to ensure that the level of resources requested is appropriate for the proposed research and also that any additional technical considerations have been captured prior to submission e.g. software licences. The process is slightly different for HPCx and HECToR, with different computing application/technical assessment forms for

each service. Please ensure that you use the correct form for the service that you are applying for time on.

HPCx applications
The Principal Investigator should submit a draft case for support together with the HPCx application form to the HPCx service (support@hpcx.ac.uk) so that a technical assessment can be undertaken, the form can be found by following the link below:

http://www.epsrc.ac.uk/Forms/Applicant/HPCxApplicationForm.htm

HECToR applications
The Principal Investigator should submit a draft case for support together with the HECToR application form to the HECToR service (support@hector.ac.uk) so that a technical assessment can be undertaken; the form can be found by following the link below:

http://www.hector.ac.uk/howcan/admin/apply/form.doc

For both services
The completed technical assessment will normally be returned to the PI within two weeks of submission to the relevant help desk for each service, although if the reviewer has concerns about the project, it may take extra time to address these with the PI. To speed up the technical assessment process, the completed computing application form and draft project case for support should be sent to the service electronically.

3.2 How to apply for Computer Resource in Support of an EPSRC Research Proposal (Class 1a access)

Prior to submission to EPSRC, Principal Investigators should obtain a technical assessment of their research proposal as described in section 3.1

After the technical assessment has been carried out by the service the full research proposal, together with the HPC application form (Sections 1 and 2), should be submitted through the Je-S portal. The HPC resources form (Section 1) and completed technical assessment (Section 2) must be uploaded as **one** pdf file.

Assessment of the proposal will be via the responsive mode process, or by the assessment procedure for the call for proposals applied to.

3.3 How to apply for Direct Access to the National Service (Class 1b on technical assessment form)

This access mechanism is for access to HECToR only.

Prior to submission to the Research Councils, Principal Investigators should obtain a technical assessment of their research proposal as described in section 3.1.

The proposal form for Class 1b access can be found by following the link below:

http://www.hector.ac.uk/howcan/admin/apply/documents/HECToR_RAP_application_form.doc

There is no limit on the number of AUs that can be applied for through class 1b access. However, applicants should note that there will be up to a maximum number of AUs available to award at each panel, subject to the quality of the proposals received.

The proposal form, together with the completed technical assessment (sections 1 and 2), should be emailed to HectorRAP@epsrc.ac.uk.

At each meeting, the RAP will produce a rank ordered list of proposals in priority order for access. The assessment criteria are:

- Scientific quality of the proposal.
- Technical suitability of the proposed work for HECToR.
- Is the proposed work capability computing, or will it enable the PI to prepare for capability computing?
- Track record in computational science and engineering of the applicant.
- Added value of access to HECToR through this mechanism.

The decision of the cut off point on the rank ordered list rests with the HECToR Service Manager.

Upcoming RAP deadlines
The Resource Allocation Panel meets every 4 months. Upcoming panel dates and their corresponding closing dates are given below. Applicants will be notified of the decision within 1 week of the panel meeting.

Successful applicants should then contact support@hector.ac.uk to confirm the start date of their access. The start date **must** be within one month of the panel date and resources **must** be used within six months of the start date.

Dates of the Panel meetings and details of closing dates for applications to the next Panel will be published here as soon as the Panel dates have been confirmed.

3.4 How to apply for Class 2a access
This access mechanism is for access to HECToR only.

Prior to submission to the Research Councils, Principal Investigators should obtain a technical assessment of their research proposal as described in section 3.1

Applications for this class of activity will only be accepted for assessment by EPSRC if they are accompanied by a positive technical assessment from the HECToR service.

The technical assessment, together with a brief (up to 2 sides) case for support, should be emailed to the HECToR Service Manager, Dr Dai Jenkins: david.jenkins@epsrc.ac.uk

3.5 How to apply for Class 2b access
This access mechanism is for access to HECToR only.

Researchers should apply for Class 2b access if they wish to apply for DCSE but do not current have access to HECToR. Applicants will be able to request a maximum of 400,000 AU in support of their proposal from the HECToR Service Manager. HECToR time will be released on confirmation of DCSE support from NAG.

Requests should be emailed to the HECToR Service Manager, Dr Dai Jenkins: david.jenkins@epsrc.ac.uk

Details of how to apply for DCSE can be found by following the link below: http://www.hector.ac.uk/cse/distributedcse/

4. Computing Resources

Computing resources on HPCx and HECToR are awarded in Allocation Units (AUs). 1 AU is equivalent to a 1 gigaflop/s processor running for 1 hour. Only the computing time resources requested are used to calculate the notional costs.

HPCx resources

When requesting HPCx resources as part of a research proposal, the PI should complete the HPCx application form, which includes a table to specify the expected resource usage for each service component for each six months of the project. At the start of a research grant, the PI (or their designated project manager) will be asked by HPCx to update this computing resource profile to form their "capacity plan". Although the six monthly profiles are not binding and the research group can use their resources at any time, subject to availability, PIs will be requested to keep their capacity plan up-to-date (through a WWW interface) as their research requirements change.

HECToR Resources

The HECToR service will be delivered in three phases and each phase will have both a vector and a scalar component. HECToR is currently in Phase 2a. Phase 2a will be available until March 2010 and consists of a 208 Teraflop/s scalar system, with a 2 Teraflop/s vector system. Phase 2b will be available from March 2010 and will consist of a 338 Teraflop/s scalar system and a 2 Teraflop/s vector system (quoted figures are peak performance). Phase 3 will be available from Oct 11 – Sep 13. The computing hardware for Phase 3 will not be procured until 2010, but the system will have a minimum size of 500 Teraflop/s (scalar). The notional cost of the resources requested has been calculated on the cost of each Phase and the planned usage of the service over these three phases. One Teraflop/s computing resource on a vector system is eight times more expensive than one Teraflop/s computing resource on a scalar system. The notional cost reflects this difference.

When requesting HECToR resources as part of a research proposal, the researcher will complete the HECToR application form, which includes a table to specify the expected resource usage on each type of system (scalar or vector) over the three Phases. ***Note, due to the fact that the per AU cost for both Scalar and Vector systems will change over the duration of the service, and that researchers may choose to apply for a mixture of Vector and Scalar components in their applications, the notional costs will have to be determined manually and entered into Je-S. This can be done by multiplying the number of AUs requested in each phase by the notional AU cost (Scalar and/or Vector) for that phase.***

The AU costs for each system and phase of HECToR can be found on the HECToR website at: http://www.hector.ac.uk/howcan/admin/costs/, which also gives further information on how these costs have been determined and details non-partner rates for HECToR. Whilst every effort is made to ensure that the details on this page are kept up to date it is recommended that all resource requests should be confirmed with the Service prior to submission of the

proposal to the council. If you have any questions regarding the amount of compute resource needed then please contact the CSE support service via the HECToR helpdesk.

Note that 'AU' is not a recognisable 'unit' on Je-S so the actual award letter for class 1a projects will say 'hours'. However, it does in fact mean 'AUs', and the time has been priced accordingly. Whilst researchers will be encouraged to use the resources that they requested for each Phase in the relevant Phase, if resources remain at the end of that Phase and the grant continues into the next Phase, they will be allowed to carry them across as long as they do not exceed the overall total level of resources awarded for the grant.

All researchers that are awarded compute time on HECToR will also have access to computational science and engineering support and training from NAG Ltd to assist them in porting and optimising their code onto the system. On receipt of their award letter, the PI is strongly advised to contact the service to discuss their requirements in this area.

5. Consortium Model

A consortium is defined as a:

"*Collection of research groups with a shared interest in developing and exploiting common computing code or computational techniques, or research groups working in a similar scientific area.*"

EPSRC funding for computing resources can be provided as part of a research grant to enable the participants to operate as a consortium, including funding for travel to consortium coordination meetings etc, and perhaps also funding for staff to carry out computational development work.

If the researcher would like to join or form a new consortium it is wise to check with the appropriate Programme Head/Portfolio Manager who can provide guidance on whether the research proposal should be incorporated into an existing consortium or whether to initiate a new consortium.

If the intention is to link a research proposal to a consortium, it is important to try and match the timeframe of the proposal and consortium for ease of final reporting. All decisions must be justified in the final report.

6. Software support

Software support is important for the next generation of computer architectures and proposals for computing time can seek funding for support and optimisation on their individual grants. Support can be a dedicated PDRA at a high performance computing centre (such as Daresbury), a HEI, as payment for a support service as a cost under exceptional items or HPCx resources for training and support.

Proposals that are awarded compute time on HECToR will have access to training and Computational Science and Engineering (CSE) support provided by NAG Ltd. Training will be at no cost to the applicant on an as required basis and available

to all users of the service, but the applicant should request sufficient travel expenses to attend such courses in their proposal. In addition to standard CSE support NAG also facilitates a distributed CSE support function to provide access to in depth support for a consortium, group or grant. The distributed CSE support will be controlled by NAG Ltd and awarded through separate peer-reviewed calls, only assessable to those researchers with current grants on HECToR funded by BBSRC, EPSRC and NERC. The cost of such support should not appear on the grant proposal.

7. Contacts

HPCx and HECToR - Liz Sim, James Clerk Maxwell Building, King's Buildings, University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ. Tel: 0131 650 5029 e-mail: support@hpcx.ac.uk or support@hector.ac.uk.

Enquiries regarding CSE will be forwarded from the Central helpdesk to the appropriate contacts.

EPSRC – Dai Jenkins, Tel 01793 444002, e-mail: David.Jenkins@epsrc.ac.uk, EPSRC, Polaris House, North Star Avenue, Swindon, Wilts SN2 1ET

Class 1b application enquiries – Sarah Fulford, Tel 01793 444 122, e-mail Sarah.Fulford@epsrc.ac.uk, EPSRC, Polaris House, North Star Avenue, Swindon, Wilts SN2 1ET