

Please note that you must read the full Call document for guidance before submitting your proposal

Resource Allocation Panel (RAP): Open access to Tier-2

Call type: Invitation for proposals

Closing date for applications to EPSRC: 16:00 on 12 October 2017

Closing date for the technical assessment: 16:00 on 21 September 2017

Resource Available: Please find the total amount of resource available at each centre listed in Annex 2.

How to apply: An application form and an approved Technical Assessment should be submitted to EPSRC.

Assessment Process: Applications to this call are not subject to postal peer review and will be reviewed and prioritised directly by a Resource Allocation Panel (RAP) at the appropriate Tier-2 Centre.

Key Dates:

Activity	Date
Technical Assessment deadline	16:00 on 21 September 2017
Closing date for application submissions	16:00 on 12 October 2017
Panel meeting	November 2017
Project start date	November 2017

Additional information: Applications to this call can request Tier-2 computing resource for a maximum duration of one year only. Applicants who wish to apply to the GW4 centre should apply for 3 months access in the first instance unless otherwise justified.

Contacts:

A full list of contact details for each Tier-2 Centre is available in Annex 3.

For any other queries please contact Katherine Freeman (ARCHERRAP@epsrc.ac.uk).

Resource Allocation Panel (RAP): Open access to Tier-2

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Related themes: Research infrastructure

Summary

The Tier-2 layer of HPC forms a vital part of an integrated e-infrastructure landscape; it addresses the gulf in capability from a local university system to ARCHER, the UK national Supercomputer.

In 2016, EPSRC recognised that the Tier-2 infrastructure needed to be refreshed and reinvigorated to ensure that it continued to be fit-for-purpose in the rapidly changing e-infrastructure landscape.

EPSRC has invested a total of £20 million in six new Centres. Please find further information on the centres here:

<https://www.epsrc.ac.uk/research/facilities/hpc/tier2/>

This is a pilot call for applications to access **five** of the new Tier-2 HPC facilities through the Resource Allocation Panel. The five facilities available to access through this call are: Cirrus, GW4, CSD3, HPC Midlands +, and JADE. For details on how to access The Materials and Molecular Modelling Hub (MMM Hub) please see their website: <https://mmmhub.ac.uk/2017/06/14/access/>. The total amount of resource available at each centre through this call is listed in annex 2 and this will be allocated subject to the quality of the proposals.

Background

EPSRC is offering open access to **five** Tier-2 HPC facilities through this call for proposals. The five facilities users can access through this call are: Cirrus, GW4, CSD3, HPC Midlands +, and JADE. Further details on each of these centres can be found in annex 1. For details on how to access The Materials and Molecular Modelling Hub (MMM Hub) please see their website: <https://mmmhub.ac.uk/2017/06/14/access/>.

Users can request significant amounts of computing resource over a maximum one-year period through this call. Applicants who wish to apply to the GW4 centre should apply for **three** months' access in the first instance unless otherwise justified because this is an experimental system.

The aim of this call is to:

Provide access to our national Tier-2 HPC facilities for adventurous high-risk, high-reward projects that will benefit from the diversity of computing architectures available at Tier-2.

A non-exclusive list of eligible projects includes:

- Short computational projects that do not warrant a full grant application;
- UK led collaborative projects with international and/or industry partners;
- Joint applications from students (as Co-Is) with proven HPC experience and their PIs;
- Projects that link consecutive standard grant applications or that aid the preparation of a grant or fellowship application;
- Extended feasibility studies and trialling application developments at scale;
- High-risk, high-reward projects that would benefit from using novel architectures.

Applications to the Resource Allocation Panel should lie within the remit of EPSRC although proposals in multidisciplinary areas will be considered. Please note that **the Tier-2 centres reserve the right to reject proposals which lie outside the remit of EPSRC**. If you are unsure about eligibility, please contact EPSRC before preparing your application.

For more information about EPSRC's portfolio and strategies, see our website:

<http://www.epsrc.ac.uk/research/ourportfolio/>

For more information about EPSRC's Tier-2 HPC Strategy, see our website:

<https://www.epsrc.ac.uk/files/research/tier2hpcstrategy/>

Resources available

Applications to this call can request computing resource only for a maximum duration of one year. Applicants to the GW4 centre should apply for **three** months of access in the first instance unless otherwise justified because the machine will initially be used for evaluation rather than a production service. Technical details about each centre can be found in annex 1.

Although there is no limit to the number of compute units which can be applied for, **there is a limit to the total amount of resource available** against this call. A full list of available resource at each centre is listed in annex 2.

Applicants with large resource requirements are encouraged to get in touch with the named contact in annex 3 before submission.

Since this type of computer access is not intended to replace full peer reviewed standard grant access, full economic costs for projects cannot be requested; only Tier-2 computing resource is available through this mechanism. Please also note that Tier-2 centres will expect users to build their own software but will provide support where possible. Any resource allocated is for immediate use and the **start date of the proposal must be within one month of the panel date** (see Call Schedule).

Please note that we do not generally grant extensions of a RAP project and any compute units which have not been used by the end of the project will be lost.

Resources for all projects will be divided into quarters and any unused resource in any quarter will be lost. It is therefore imperative that applicants are well-prepared and only request an allocation they can realistically use in the allocated period. This should take into account queuing times, potential issues with newly ported codes, scheduled maintenance periods and the time to respond to intermediate results. Please note that if you are applying to access CSD3, for a project which is longer than three months, resources will be divided pro rata into quarterly allocations unless the application requests and provides justification for a different division of resources. **Please do not hesitate to contact the Tier-2 Centre at an early stage if any computational issues occur.**

Exciting high-risk/high-reward research is strongly encouraged, but careful consideration is needed to ensure that the requested allocation is appropriate and can realistically be used within the project duration.

As a pump priming opportunity for new users Tier-2 centres may offer instant access to give new users the opportunity to test the systems for their purposes and work towards a fully peer reviewed application, either via a standard grant or via this Open Access call. For example CSD3 has a light touch access mechanism for Proof of Concept and Pump Priming applications which are designed to allow users to gather evidence to support large applications for resources. More details about this can be found at <http://www.csd3.cam.ac.uk/> and you are welcome to contact Prof Payne (resources@csd3.cam.ac.uk) to discuss these access mechanisms.

Please note that if you are from an institution that is a named member of a Tier-2 Consortium and you wish to use that consortiums machine, you should apply for resources by contacting the centre directly. However if you wish to access another Tier-2 machine you are eligible to apply for resource through this call.

HEC Consortia members are eligible to apply through this call, with the exception of UK Car-Parrinello Consortium (UKCP) and Material Chemistry Consortium (MCC) members who would like to access the MMM Hub. If you are a member of one of these consortia please contact your consortia directly and find details of how to access the MMM Hub here: <https://mmmhub.ac.uk/2017/06/14/access/>.

Please consider carefully if Tier-2 is the appropriate resource for your proposal. If your project would be better placed at a Tier-1 or Tier-3 resource, please contact the respective Tier-1 centre or local University directly.

Please note that you can apply to the following centres through this call: Cirrus, GW4, CSD3, JADE and HPC Midlands+. For details on how to access the The Materials and Molecular Modelling Hub (MMM Hub) please see their website: <https://mmmhub.ac.uk/2017/06/14/access/>.

Equipment

Equipment is not available through this call.

For more information on equipment funding, please see: <https://www.epsrc.ac.uk/research/facilities/equipment/>

Eligibility

Only individuals eligible to hold a full EPSRC grant can apply to the Resource Allocation Panel. This specifically implies that students wishing to access HPC resources through this route must obtain commitment for support by an eligible PI.

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

<https://www.epsrc.ac.uk/funding/howtoapply/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/>

Only one application per PI or Co-I is permitted in each round.

How to apply

A two-stage application process will be used.

Stage 1- Applicants must submit a Technical Assessment to the appropriate contact at the centre they wish to apply for access to, along with a short project description. This TA form will be assessed by the contact at the centre and returned to the applicant. A list of contact details for each centre can be found in annex 3.

Stage 2- Applicants must then submit the following documents to the EPSRC Call page:

- 1) Completed and approved Technical Assessment
- 2) Application Form
- 3) A one-page diagrammatic workplan

Stage 1 Tier-2 technical assessment

Applicants must submit a completed **technical assessment together with their application** in order for it to be considered by the panel. This additional step is important to ensure that the level of resources requested has been appropriately scoped and that all technical requirements have been considered prior to submission.

In order to obtain a technical assessment, applicants should submit a short project description together with a technical assessment form (available for download from the EPSRC call page at <https://www.epsrc.ac.uk/funding/calls/tier2openaccess/>) to the contact at the centre they wish to apply to listed in annex 3, prior to **16:00 on 21 September 2017**.

Please make sure the subject header of your submission email states that this is a "Tier-2 submission".

At the Technical Assessment stage if your application is deemed to be more technically appropriate for access at another Tier-2 Centre or ARCHER, then your

TA form may be passed on to that HPC facility to assess and you will be encouraged to submit an application for access at that centre.

The completed technical assessment will normally be returned to the applicant promptly, although if the reviewer has concerns about the project, it may take extra time for these to be addressed. **EPSRC and the service cannot be held responsible for applications that miss the final deadline if the applicant has not met the deadline specified above for submission of the technical assessment.**

Stage 2 Application form

Applicants should download the application form from the EPSRC call page: <https://www.epsrc.ac.uk/funding/calls/tier2openaccess/>

When completing your application form you should take into account the assessment criteria given below (see Assessment Criteria) and consider the broad expertise of the panel (see Assessment Process). **Applications submitted on an incorrect form will not be considered.** No additional letters of support are allowed.

Submitting the application

Provided the technical assessment endorses the proposal, **applications should be sent together with the completed technical assessment** and a one-page diagrammatic workplan directly to the call page (<https://www.epsrc.ac.uk/funding/calls/tier2openaccess/>) before the call deadline. Please submit all documents as a single PDF file.

Guidance on writing application

Track Record (max one page): Provide details of the applicant(s) track record in computational science and engineering, porting, developing and using codes, on HPC facilities. Highlight any previous publications or other scientific outputs arising from HPC work relevant to this application. If you are new to HPC, how do you plan to involve partners to ensure the necessary computing expertise is guaranteed? Please include any other information you think is relevant to demonstrate applicant(s) suitability to undertake this work.

If your project involves collaboration with an international or industrial partner please include any information you feel is relevant regarding their expertise and your collaboration with them.

Other resources associated (max ½ page): State details of any additional financial and/or technical support for this or other research projects relevant to this application. As this proposal is for computing resources only, applicants should give details of how any other necessary resources for the project (e.g. staff time) will be made available.

Objectives (max ½ page): Briefly list the main objectives of the proposed research, written for a generalist scientific audience. Explain how Tier-2 will help you to meet these objectives.

Science Case (max two pages): Describe your proposed research explaining clearly the novelty and timeliness of the work. Explain how it will deliver a high-

quality scientific output, or lead to results that will ultimately enable high-quality scientific research.

Please explain why the particular Tier-2 centre is the most appropriate resource for this work, rather than other national, tier-2 or local (university) resources.

Resources Management (max one page): Please state the requested number of compute units, memory, storage; as approved by the technical assessment. Please state how much storage space you require. It is important that you ensure a timely start and finish of the project as well as efficient use of the granted allocation over the requested time period. No extensions will be granted and any resources which have not been used by the end of the period will be lost. If the work has particularly novel elements that could be considered high risk - high reward, please indicate how the risks will be managed.

Explain how you plan to use and manage the allocated resources and describe the staff resources available to complete the project. Please remember that the total number of compute units allocated through this process is limited. If you are applying for a comparatively large amount of compute resources, you need to demonstrate that your code(s) can make optimal use of this resource – e.g. by providing detailed, relevant, benchmarking and scaling data. It is important that you ensure a timely start and finish of the project as well as efficient use of the granted allocation over the requested time period. (Please note, the Resource Allocation Panel can recommend a reduction in units or time awarded if the original request is not fully justified).

Assessment

Assessment process

Stage 1- Technical Assessment

Technical Assessment forms will be reviewed by technical reviewers e.g. a Research Software Engineer, at the Tier-2 Centre you have submitted your Technical Assessment form to. The Technical Assessment stage is carried out to ensure that the level of resources requested have been appropriately scoped and that all technical requirements have been considered prior to submission of an application to EPSRC. Applicants will receive comments made by technical reviewers on the Technical Assessment form and can respond to these by amending the technical aspects of their forms before the Technical Assessment is approved.

At the Technical Assessment stage if your application is judged to be more appropriate for access at another Tier-2 Centre or ARCHER, then your Technical Assessment will be passed on to that HPC facility for review and you will be notified and encouraged to submit an application to that centre. The aim of this step is to coordinate resource allocation across HPC centres in the UK and allow the transfer of applications which are more appropriate to another Tier-2 system or to ARCHER. Therefore proposals which the technical reviewer deems more suited to a different HPC machine may be awarded HPC time on ARCHER or another Tier-2 machine.

Stage 2- Resource Allocation Panel

Applications to this call are not subject to postal peer review and will be reviewed and prioritised directly by a Resource Allocation Panel (RAP). Brief feedback will be provided to applicants after the panel and the panel can recommend if an applicant can resubmit to this call.

The RAP is selected to comprise a broad cross section of HPC users from disciplines within engineering and the physical sciences.

Once applications have been received by EPSRC they will be directed to the appropriate Tier-2 centre and will be assessed by a RAP. There will be one panel meeting at each Tier-2 centre. At the panel meeting, the RAP will rank the submitted proposals in priority order for allocation. Each centre will then decide on the total number of compute units and time awarded.

After the RAP panel there will be a follow-up Chairs meeting. This meeting will consist of Panel Chairs from each Tier-2 Centre RAP and the ARCHER RAP Chair. The purpose of this panel is to gather feedback on the application and peer review process for this pilot call. If necessary, this meeting may also discuss any proposals where a decision could not be reached at the RAP meetings or Technical Assessment stage about whether an application was appropriate for a particular HPC facility. Any such proposals will be ranked within the priority list for the HPC centre which is deemed most suitable for that proposal and the applicant may be awarded time at a different HPC facility. Please note it is EPSRC's expectation that all decisions of this nature will be made at the Technical Assessment stage and there may not be any proposals that will need to be discussed at this meeting.

Please note this is a pilot call for access to these facilities and EPSRC will be reviewing this process for access.

Applicants will be notified of the outcome of the panel as soon as possible after the meeting. **Successful applicants should then email the contact detailed in annex 2 to confirm the start date of their project.**

Assessment criteria

The assessment criteria used by the panel to rank proposals are:

- **Scientific quality:** What is the quality, importance, novelty and timeliness of the proposal in terms of the scientific research proposed? To what extent will the proposal deliver a high quality scientific output, or lead to results that will ultimately enable high quality scientific research? To what extent, is the proposed work exploring novel and new ideas that may have a high risk, high reward element?
- **Appropriateness and Technical suitability:** What is the technical suitability of the proposed work for the facility? Is the facility the best or only UK system on which this research can be conducted?
- **Applicant(s):** Is this the appropriate team to undertake the research proposed? What is the applicant(s)' track record in computational science and engineering, porting, developing and using codes, on HPC facilities? What is their track record of publishing in this area? If the applicants are relatively new to HPC, are appropriate support mechanisms in place to guarantee efficient use of the allocated resource?

- **Resources and Management:** Is the level of requested resource appropriate and well justified? Does the proposal contain a clear work plan that justifies the requested time? Is there sufficient staff time allocated to do this work? Is the project adequately managed, including potential risks? To what extent are the risks involved with the project appropriate and adequately managed?

Feedback

As the proposals will not be postal peer-reviewed, brief feedback will be given to each applicant after the Resource Allocation Panel. Furthermore the panel can recommend invited resubmissions.

Moving forward

Submissions to this call will **not** count towards the Repeatedly Unsuccessful Applicants Policy. Further information about the policy can be found at: <https://www.epsrc.ac.uk/funding/howtoapply/basics/resubpol/rua/>

Applicants will be notified of the outcome of the panel within one week of the meeting.

Key dates

Activity	Date
Technical Assessment deadline	16:00 on 21 September 2017
Closing date for application submissions	16:00 on 12 October 2017
Panel meeting	November 2017
Project start date	November 2017

Contacts

For further information about this call, please contact:

ARCHERRAP@epsrc.ac.uk

Change log

Name	Date	Version	Change
Katherine Freeman	22/06/2017	0.1	n/a
Katherine Freeman	11/07/2017	0.2	Amended following comments from Tier-2 centres

Name	Date	Version	Change
Katherine Freeman	02/08/2017	0.3	Amended following comments from Peer Review

Annex 1-Technical Details for Tier-2 Facilities

Please find details about each of the Tier-2 facilities below.

Cirrus HPC Service from EPCC (Cirrus)

System: HPE/SGI ICE XA Cluster

Interconnect: FDR Infiniband

Cabinets: 2 SGI E-Cells. Each E-Cell consists of 2 compute node racks and a cooling rack.

Compute Nodes: 280 dual CPU nodes

Processor: Each node has two 2.1 GHz, 18-core Intel Xeon E5-2696

(Broadwell) series processors. Each 18-core processor has 128 GB local memory.

Further details about Cirrus can be found here:

<http://www.cirrus.ac.uk/about/hardware.html>

GW4 Tier 2 HPC service (GW4)

System: Isambard (Phase 1)

Interconnect: EDR InfiniBand

Storage: Cray Sonexium 3000, providing a total 480TB capacity presented using Intel IEEL Lustre

Compute Nodes: 4 * dual NVIDIA P100 and 8 * Intel Phi KNL

Processor: NVIDIA: 2 x Intel Xeon E5-2694 v4 (2.1Ghz /18c Broadwell / 512GB memory) and 2x NVIDIA Tesla P100 Pascal accelerators; KNL: 1 Intel KNL 7210 1.3GHz / 64c processors, 768 GB memory (using 16GB DR4-2400 MHz DIMMS)

Cambridge Service for Data Driven Discovery (CSD3):

System Name	Specification
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Peta4-Skylake	Compute Node Type1 (384)
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	Processor: 2 x Intel Xeon Skylake 6142 processors, 2.6GHz 16-core
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	Memory: 384GB
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	Interconnect: Intel OmniPath
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	Compute Node Type2 (384)
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	Processor: 2 x Intel Xeon Skylake 6142 processors, 2.6GHz 16-core
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Memory: 192GB

Interconnect: Intel OmniPath

Peta4-KNL

Compute Node (342)

Processor: KNL 7210

Memory: 96GB

Interconnect: Intel OmniPath

Wilkes2-GPU

Compute Node (90)

Processor: 1 x Intel Xeon E5-2650 v4 2.2GHz 12-core processor

GPU: 4 x Nvidia P100 GPU 16GB

Memory: 96GB

Interconnect: EDR InfiniBand

Further details about csd3 can be found here: www.csd3.cam.ac.uk

HPC Midlands +

512 compute nodes in Huawei X6000 quad-node chassis, each with:

- 28 cores, in the form of two Intel Xeon E5-2680v4, and
- 128 GB of memory

giving a total of 14,336 cores and 64 TB of memory.

1 Petabyte of disk storage, delivered via GPFS from four storage nodes.

An EDR Infiniband high-performance internal network. This is structured hierarchically, with islands of 27 nodes (756 cores) connected at full EDR bandwidth, and the islands are then connected to the core of the network at one-third bandwidth.

5 OpenPOWER compute nodes, each with 20 cores and 1 TB of memory.

One of the OpenPOWER nodes also has two Nvidia GP100 GPGPU cards, connected via NVlink.

Please find further details about HPC Midlands + here: <http://www.hpc-midlands-plus.ac.uk/about/system-description/>

The National GPU facility for machine learning, molecular dynamics, and data science research- JADE

System: 22 NVIDIA DGX-1 Deep Learning Systems

Processor: 8 of NVIDIA's newest Tesla P100 GPUs

Interconnect: NVIDIA's high-speed NVlink interconnect.

Storage: 4 TB of SSD for machine learning datasets. Over 1PB of Seagate ClusterStor storage

Software: optimized versions of major machine learning software packages such as Caffe, TensorFlow, Theano and Torch

Please find further details about JADE here:

<http://www.arc.ox.ac.uk/content/jade>

The Materials and Molecular Modelling Hub (MMM Hub)

The HPC facility that the MMM Hub hosts is known as Thomas, a 17,000 core machine based around Lenovo 24 core Intel x86-64 nodes.

Please see their website: <https://mmmhub.ac.uk/>

Annex 2- Resources available at each Tier-2 centre

1. Cirrus

A total of 20 MCPuH is available through this call.

2. GW4 Isambard Service

The GW4 Isambard is making 25% of its compute cycles available to ESPRC eligible funded research. This is an evaluation service comprised of multiple advanced architectures housed within the same environment to enable architecture comparison across the latest Intel Xeon Phi, NVIDIA Pascal P100 GPU, and from 2018, ARMv8 64-bit processors. Isambard Phase 1 provides access to a Cray CS400 comprising Intel Xeon Phi KNL and NVIDIA Pascal P100 nodes with a Cray Sonexium 3000 storage system. Phase 1 specifications are:

- **Four** NVIDIA nodes using 2 x Intel Xeon E5-2695 v4 (2.1GHz / 18c Broadwell, 512GB memory) with 2 x NVIDIA Tesla P100 Pascal GPUs.
- **Eight** Intel Xeon Phi KNL nodes using 1 x Intel KNL 7210 1.3GHz 64c processors, 768GB memory (using 6 *16GB DR4-2400 MHz DIMMS)
- Storage is the Cray Sonexium 3000, providing a total 480TB capacity, presented using Intel IEEL Lustre using EDR InfiniBand.
- Operating System uses RedHat Linux and the Altair PB Professional Job Scheduler.
- Development Software environment includes the Cray Programming Environment and ARM/Allinea's DDT (256 license token).
- Training and 2.0FTE RSE Support Expertise available to assist researchers in installing applications on the service and investigating performance optimisation in collaboration with Cray and ARM64 as part of the ARM64 Centre of Excellence.
- Phase 2 is being installed during H1/2018 and will introduce the ARMv8 64-bit processors. In advance of this, early pre-production ARM silicon is being investigated and could be integrated into the solution by Q4/2017, but would be subject to NDA access requirements due to the early pre-production release nature of the processor.

Please note, due to the evaluatory nature of the GW4 service, project times are not envisioned to be more than **three** months unless extended times are justified in the proposal.

Please see the GW4 website for further information: <http://gw4.ac.uk/>.

3. CSD3

The following resource is available through this call:

1. 39405906 Skylake Core hours, with a minimum usage of 2000000
2. 577235 P100 GPU hours, with a minimum usage of 17000
3. 548373 KNL hours, with a minimum of 16000.

Users can request significant amounts of resource (from a minimum of 3% or 5% dependent on the pool)

For more information visit: www.csd3.cam.ac.uk

4. **JADE** - The amount of machine time available through this call will be up to 200k GPUh (around 15% of the GPUh available).
5. **HPC Midlands +** - 15% of the HPC Midlands machine will be available through this call.
6. **MMM Hub** - Further details on how to access this system and how much resource is available can be found here:
<https://mmmhub.ac.uk/2017/06/14/access/>

Annex 3 - Contacts at each Tier-2 Centre

Cirrus - for all queries please email epcc-support@epcc.ed.ac.uk

MMM Hub - for all queries please email rc-support@ucl.ac.uk

CSD3 - for general queries on access please email Prof Mike Payne (resources@csd3.cam.ac.uk). For Technical Assessment submissions please email: Mr Filippo Spiga (rse@csd3.cam.ac.uk)

GW4 "Isambard" Tier-2 Site - for general queries please see the website <http://gw4.ac.uk/isambard> or email GW4@cardiff.ac.uk. For technical Assessment submissions please email gw4@cardiff.ac.uk. For application specific questions, please contact Professor Simon McIntosh Smith (cssnmis@bristol.ac.uk) copying Dr. Christine Kitchen (kitchenca@cardiff.ac.uk) so we can escalate your enquiry accordingly.

HPC Midland+ - for all queries please email research-computing@lboro.ac.uk

JADE - for all queries please email support@arc.ox.ac.uk