DiRAC Resource Allocation Committee
Call 13.5: Special Call for Proposals for DiRAC-3 Resources
Guidance notes for Applicants

Contents

1. Introduction

1.1. The DiRAC (Distributed Research utilizing Advanced Computing) facility is the STFC national HPC resource for the UK astronomy, cosmology, particle physics and nuclear physics communities. This Special Call of the Resource Allocation Committee will cover computational resources on the new DiRAC-3 systems during a 6 month period from 1st October 2021 to 31st March 2022. A summary of the hardware which will be available in this call can be found in the table in Annex 1.
Information on the HPC services that DiRAC offers can be found at http://dirac.ac.uk.

1.2. This Call is in addition to the 14th RAC Call which will open later in the year for allocations starting from 1st April 2022.

2. DiRAC Resource Allocation Committee

2.1. The DiRAC Resource Allocation Committee (RAC) was established to oversee the time allocation for DiRAC project proposals. The membership of the RAC is available at https://dirac.ac.uk/resource-allocation-committee/. To maximise the quality of the scientific output of DiRAC, the allocation of time will be determined via robust, transparent peer review. The RAC has two sub-panels, one for Particle Physics & Nuclear Theory and one for Astronomy & Cosmology, which will consider the proposals within their respective remits. A meeting of the RAC attended by representatives from both Sub-Panels will determine the overall allocation of DiRAC time across the whole portfolio of proposals.

3. Call Closing Dates

3.1. The closing dates for proposal submissions is as follows:

Expressions of Interest: Monday 14th June 2021, 17:00
Full proposal (Scientific and Technical cases): Wednesday 30th June 2021, 17:00

4. Enquiries

4.1. All Call application forms and documentation can be found on the DiRAC website. Enquiries should be directed as follows:
- RAC process and remit: STFC Swindon Office DiRACRAC@stfc.ac.uk
- Technical questions: dirac-support@epcc.ed.ac.uk
- Direct allocations or discretionary requests: DiRAC Director, Prof Mark Wilkinson (miw6@leicester.ac.uk)

5. Equality, Diversity and Inclusion

5.1. In line with the UK Research and Innovation Diversity Principles, STFC expects that equality and diversity is embedded at all levels and in all aspects of research practice. We are committed to supporting the research community in the diverse ways a research career can be built with our investments. This includes career breaks,

support for people with caring responsibilities, flexible working and alternative working patterns. With this in mind, we welcome applications from academics who job share, have a part-time contract, need flexible working arrangements or those currently committed to other longer, large existing grants. Please see our [Equality and Diversity webpages](#).

6. Impact of Covid-19 Pandemic

6.1. UKRI recognises that the COVID-19 pandemic has caused major interruptions and disruptions across our communities and are committed to ensuring that individual applicants and their wider team, including partners and networks, are not penalised for any disruption to their career(s) such as breaks and delays, disruptive working patterns and conditions, the loss of on-going work, and role changes that may have been caused by the pandemic.

6.2. Reviewers and Panel Members will be advised to consider the unequal impacts of the impact that COVID-19 related disruption might have had on the track record and career development of those individuals included in the proposal and will be asked to consider the capability of the applicant and their wider team to deliver the research they are proposing. Where disruptions have occurred applicants can highlight this within their application, if they wish, but there is no requirement to detail the specific circumstances that caused the disruption.

6.3. UKRI acknowledges that it is a challenge for applicants to determine the future impacts of COVID-19 while the pandemic continues to evolve. Applications should be based on the information available at the point of submission and, if applicable, the known application specific impacts of COVID-19 should be accounted for. Where known impacts have occurred, these should be highlighted in the application, including the assumptions/information at the point of submission. There is no need to include contingency plans for the potential impacts of COVID-19.

6.4. Reviewers will receive instructions to assume that changes that arise from the COVID-19 pandemic, post-submission, will be resolved and complications related to COVID-19 should not affect their scores.

6.5. Where an application is successful, any changes in circumstances that affect the proposal will be managed as a post-award issue.

7. Eligibility

7.1. Each proposal must identify a Principal Investigator (PI) who has overall responsibility for the delivery of the proposed research and will act as the point of contact for all STFC, DiRAC and RAC communications.

7.2. In line with STFC's research grant conditions the PI must be either a) resident in the UK, or b) be employed by an overseas Research Organisation approved by STFC as eligible to apply for research grant funding. The STFC eligibility criteria can be found

via this this [link](#).

7.3. We welcome proposals that represent the UK's contribution to an International Research Programme. However, it is expected the proposed research programme will enhance the UK's research outputs. Applicants are invited to submit letters of verification if the work proposed is dependent on other scientific results or being part of a large collaboration. If any projects are heavily led by international collaborators full reasons for this must be provided in the case for support. If applicants are aware of any restrictions on their ability to acknowledge the use of DiRAC resources in their publications, for example because of rules within an international collaboration, they should indicate these in their proposal. (Note that this will not affect the assessment of the proposal but will ensure that appropriate reporting mechanisms can be agreed with the PI if the proposal is successful).

7.4. Please note that if applicants hold an existing STFC Consolidated Grant this does not automatically guarantee that they will be allocated computing time on DiRAC facilities.

8. Proposal Types

8.1. Two types of proposal will be accepted to this call:

- **Uplift of an existing allocation**
  Projects with existing RAC allocations may request an uplift of up to 100% of their current allocation between October 2021 and March 2022, or 40% of the total resources on a given machine, whichever is lower. For example, in the case of a 100% uplift, the allocation for this 6 month period would then become twice the original allocation.
- **New science allocations**
  Applicants may apply for up to 80% of the new resources based on a new science case.

8.2. For both application types, it is essential that a clear management plan must be submitted to show that sufficient staff effort is available within the duration of the award to make full use of the increased allocation. Any existing projects which are under using their allocations are unlikely to be awarded an increased allocation unless there is clear evidence of a material change in anticipated usage (for example, A PDRA taking up a new post from October).

9. How to submit a proposal

9.1. **Statement of Interest**
Applicants for both proposal types must firstly complete and submit a Statement of Interest (SoI) form. This form can be found on the DiRAC website. The SoI form must be sent via email to STFC (DiRACRAC@stfc.ac.uk) by **Monday 14th June 2021.** This is to assist with Call planning. The SoI will not be assessed and you will not receive any feedback on this, but you will receive an email confirming your SoI has been

received.

9.2. **Uplift of an existing allocation**
Applicants wishing to request an uplift of an existing allocation must complete and submit the following documents listed below direct to STFC (DiRACRAC@stfc.ac.uk) by **Wednesday 30th June 2021**. The proposal documents can be found on the DiRAC website. Applicants may wish to send proposals via encrypted email.

- Scientific application form
- Technical application form – this is only needed if you are proposing to use a new code, or on a larger scale than your existing project allocation. If you will be using the same codes and on the same scale as your existing allocation you will not need to complete a new technical form as the original technical form will still be valid.
- Case for Support – this should be no longer than 2 pages. It must detail how the uplift will increase the impact of the existing allocation and explain how this is within the same science goals. A new, full case for support is not required as it is assumed that the case for support submitted for the existing allocation will still be valid.
- Management Plan – this should be no longer than 2 pages and must show that sufficient staff effort is available within the duration of the award to make full use of the increased allocation. Any existing projects which are under using their allocations are unlikely to be awarded an increased allocation unless there is clear evidence of a material change in anticipated usage (for example, a PDRA taking up a new post from October).

9.3. **New science allocation**
Applicants wishing to request resources for a new science project must complete and submit the following documents direct to STFC (DiRACRAC@stfc.ac.uk) by **Wednesday 30th June 2021**. The proposal documents can be found on the DiRAC website. Applicants may wish to send proposals via encrypted email.

- Scientific application form
- Technical application form
- Case for Support, Management Plan and Data Management Plan (please see section 9.3.1 below)

9.3.1. **Case for support**
The case for support for new science allocations must be a maximum of 6 pages and contain the following information listed below:

1) **Science justification and proposed research** (maximum 3 pages)
This should describe the proposed research programme and explain why you wish to use DiRAC. It should address the following areas:

   a. Significance of the proposed research goals with reference to the STFC Roadmap
   b. Suitability of the proposed methods / codes
   c. Justification of the resources requested

d. Suitability of the Investigator(s) for the proposed research
e. Justification of any periods of machine use in exclusive mode
f. A prioritised list of the projects within the proposal
g. Clarification of the absolute minimum time required for the proposed work, including full reasons for needing all of the time requested, why the time requested is essential for the successful completion of the project, and the scientific impact of any cuts.
h. The technical case and scientific case should both provide information explaining how intensively the proposed code will be used, and how much of the allocated time will be used by this code. This should be addressed for all of the major codes that are listed.

2) **Project Management Plan** (Maximum 2 pages)
This must describe the management arrangements of the project as detailed below:

a. The project management structure
b. Availability of sufficient staff effort to carry out the proposed research and to make full use of the allocation (a table should be included showing the estimated effort, as a percentage, that the PI and each Co-I expect to contribute to the project)
c. A description of the internal allocation process for the allocation of time to sub-projects (if applicable)
d. A work plan, with milestones against which the progress of the project will be measured
e. Publication plans
f. Project risk and mitigation analysis (include compute/storage usage, staff and technical risks)

3) **Data Management Plan** (Maximum 1 page)
Applicants are required to complete a short data management plan. This is mandatory and will be assessed in the review of the proposal by the RAC. Applicants are requested to address all points which are found in the STFC Data Management Plan (DMP) guidelines (available here). This includes which communities may have potential interest in the data being produced by their DiRAC project; how and where the data from the project will be stored; how long the data will be stored and what metadata processes will be used.
Applicants are encouraged to consult the DMPs of any collaboration they are a part of and to discuss with their universities data management units.

4) **Relevant publications** produced via DiRAC resources over the last 3 years (short annex)

5) **References** (short annex)

10. **Peer Review Process**

10.1. **Uplift of an existing allocation**
The RAC will carry out a "light touch" review of proposals requesting an uplift of an

existing allocation. This is because the science would have already been peer reviewed when the original proposal was submitted. The Panel will consider how the uplift will increase the impact of the work in the existing allocation and will refer to the original proposal and case for support to ensure the work proposed is within the same science goals (applicants do not need to provide a copy of the original proposal as STFC will already have this, so please ensure you include your RAC reference number on the scientific application form). Assuming the new proposal adequately demonstrates these points, it will be considered eligible and the RAC will use the score of the existing allocation considering the science will be the same as that within the existing proposal. This score will be used to determine the proposal's position in the overall ranking list of all proposals submitted to this call.

The technical case, if applicable, will be assessed by the DiRAC RSE team.

10.2. **New science allocation**

Proposals requesting a new science allocation will go through the following peer review process:

1) Proposals will not be sent to external reviewers but will instead be assessed by a small ad-hoc Panel which will report to the relevant Sub-Panel of the RAC, in the same way an external reviewer would provide a review of a proposal. This small ad-hoc Panel will produce a report (similar to a reviewer's report) which will be shared with applicants for their response.

2) The relevant Sub-Panel will assess the proposal in line with the set criteria, taking into consideration the review provided by the small ad-hoc Panel and the PI's response, and will provide a score for each proposal and form an overall ranking list of all proposals submitted to this call.

3) The Technical case will be assessed by the DiRAC RSE team.

11.   Assessment Criteria

11.1. Proposals will be assessed according to the following criteria (please see Annex 2):

a) Scientific Excellence (total weighting of 60%)

- Significance of the proposed research goals with reference to the STFC Roadmap
- Strategic value within the STFC programme
- National and international competitiveness and leadership
- Suitability and national/international standing of the investigator(s) for the proposed research

b) Project Management (weighting 10%) **and Data Management** (weighting 10%)

- Feasibility of project timeline considering the DiRAC resources requested and size of investigator team
- Project risk and mitigation analysis (include compute/storage usage, staff and technical risks)
- Publication plans
- Availability of sufficient staff effort to carry out the proposed research and make full use of the allocation.
- Direct response to the STFC Data Management policy guidelines

c) Technical Assessment by DiRAC RSE Team (Total weighting 20%)

- Appropriateness of the proposed architecture/machine selection

- Efficiency of resource usage and how well code(s) vectorise

d) **RAC Additional Scoring considerations** (please see Annex 3)
- Alignment of the proposal with the call guidelines.
- Full and effective usage of previous DiRAC allocations. Reasons for any under usage of previous DiRAC allocations will be taken into consideration.
- Timely submission of interim and final reports of any previous DiRAC allocation.

11.2. A score between 0 – 10 will be applied to the RAC additional scoring considerations. This will then form a percentage decrease in the overall score gained from the main criteria with a maximum of 20% decrease in score. For example, a score of 9 would produce a 2% reduction in the final score.

12. Important points to note

12.1. No single application may request more than 80% of the available time on any individual machine.

12.2. Proposals should be focused on scientifically coherent themes, but should contain sufficient technical and scientific detail. It should be noted that proposals with greater numbers of themes will generally result in poor coverage and potentially weaker reviews.

12.3. Proposals should include adequate detail to justify the requested allocation and should be written in a way that is accessible to the RAC panel, who may not be an expert in the given field.

12.4. The DiRAC resources are divided into two allocation periods covering the duration of the awards in this call (01/10/21 – 31/03/22), starting 1st October and 1st January. Successful applicants will be advised of the total amount of resources they have been allocated. The allocations for each period will be shown in the DiRAC SAFE system. Resources must be used in the allocation period to which they are assigned; they cannot be carried over to the next allocation period.

13. Code Efficiency

13.1. The aim of the RAC process is to maximise the output of high quality research by the DiRAC facility. Scientific excellence will be the primary driver for allocation decisions and the RAC will balance 'time to science' against reasonable requirements on the operational efficiency of approved projects and simulation codes. It is recognised that the cutting-edge and novel nature of research across the DiRAC community means that many DiRAC codes are under active development and may not be as efficient or scalable as more mature codes. Further, results obtained in a timely manner with a sub-optimal code will often have greater impact than results delayed by extended periods of code optimisation work. However, while it is recognised that new HPC users, or users of new codes, may not have sufficient resources or experience to provide full details of code efficiency, applicants will be required to demonstrate that their operational plan is as efficient as possible and that the architecture requested is

the most appropriate for the work.

13.2. In cases of similarly ranked proposals, applicants who demonstrate more efficient use of DiRAC resources either in terms of actual code efficiency or more efficient operational strategies will be given preference.

13.3. The resources being offered in this call are based on new CPUs (AMD Rome, Intel Icelake) and GPUs (Nvidia A100) Intel Skylake. As the new resources will not be available for scaling or efficiency tests before the closing date of this call, scaling and efficiency information based on existing DiRAC services will be accepted. *If you are able to provide data from systems using the same (or similar) hardware as the new DiRAC services, please note that your request is based on these figures.*

14.   Requesting exclusive use of a DiRAC system

14.1. Some projects may include (or may consist entirely of) sub-projects which require usage of an entire DiRAC machine, or significant fraction of a machine, for a period of longer than two days. This mode of use must be explicitly justified in the proposal, and a detailed timeline for the sub-project must be included. The technical assessment of such sub-projects will include an assessment of the efficiency of machine use.

14.2. If the request is approved, a fixed start date for the sub-project exclusive usage will be agreed to enable re-scheduling of other users to other machines during the period of unavailability. Time lost due to failure to meet the approved start deadline will not be compensated.

14.3. No more than two DiRAC machines will be operating in this mode at any one time. Where this mode of operation directly impacts on another project (e.g. due to technical requirements which mean it cannot be moved to another machine) it may be necessary to sub-divide periods of exclusive use or reserve a fraction of the cores for other projects. In cases where multiple Project proposals with overlapping scientific goals are received, if appropriate the RAC may invite the applicants to consider merging their proposals.

15.   Project Reporting

15.1. Projects requesting an uplift of an existing allocation must include details of this work in the usual annual and final report for the existing project.

15.2. Projects requesting resources for a new science allocation must submit a final report at the end of the project describing facility usage, progress against objectives, achievements and publications. You will be notified by STFC when this is due.

15.3. Failure to submit a satisfactory report will result in subsequent proposals from the group being marked down.

16.   Storage Policy

16.1. Please note the following information regarding the DiRAC Storage Policy:

Quota - an amount of disk that you cannot exceed.

Allocation - an amount of disk that you are guaranteed to have access to.

/home - this will be small and have quotas applied of, say, 10GB. This is for storing code, key input files, etc. but is not a working space.

/scratch or /work - this is the main working area available to all compute nodes and is quota'd by having separate volumes/file systems, one per project. The amount of space allocated to scratch can be over-allocated, hence it is a quota rather than an allocation. It is left to the users to manage their data within the limits of the set quota. However, each DiRAC site reserves the right to sweep of files which have not been accessed for a given amount of time. This is at the discretion of each site.

/data (medium term) - this is for storing results awaiting final post processing or on which more work may be required prior to publication and transfer back to the user's own institution. These will be quota'd to reduce the risk of significant overutilisation. Sweeping will be used here as well, as it is not a permanent archive, but will be on a much longer access time, say 9 months.

Archive: This is tape storage. Applicants must specify what data products they wish to have backed up to tape. Note that DiRAC is not currently able to provide long-term data storage/curation.

Note that not all DiRAC sites have all categories of storage types described above available. DiRAC will endeavour to assign storage aligned to the categories requested but this may not be technically possible.

Annex 1: Available resources for RAC 13.5 Special Call

Service	CPU nodes	GPU nodes	Fat nodes	Network	Storage
Data Intensive – Cambridge	268 nodes each with: o 2x 38-core Intel Icelake CPUs o 512 or 256 GB RAM **Total: 20,368 cores**	21 nodes each with: o 4x A100-80GB Nvidia GPUs o 1TB RAM o 2x 64-core AMD Milan CPUs **Total: 84 GPUs**	N/A	3:1-blocking, 200Gb/s	3.5 PB disk
Data Intensive – Leicester	200 nodes each with: o 2x 64-core AMD Rome CPUs o 512 TB RAM **Total: 25,600 cores**	N/A	N/A	3:1-blocking, 200Gb/s	4 PB disk
Extreme Scaling – Edinburgh	6 nodes, each with: o 2x AMD Rome CPUs o 256 GB RAM **Total: 768 cores**	112 nodes, each with: o 4x A100-40GB Nvidia GPUs o 2x AMD Rome CPUs o 1 TB RAM **Total: 448 GPUs**	N/A	Non-blocking, 200Gb/s	4 PB disk
Memory Intensive – Durham	360 nodes each with: o 2x 64-core AMD Rome CPUs o 1 TB RAM **Total: 46,080 cores**	N/A	2x 4TB with AMD CPUs	Non-blocking, 200Gb/s	5.3 PB disk; 20 PB tape; 1.1 PB SSD (checkpointing)

Annex 2: Scoring Matrix

Category	N/A	Unfundable	Not Competitive	Good	Excellent	Exceptional
Score	0	1-2	3-4	5-6	7-8	9-10
Scientific Case	No Science Case submitted, or at an insufficient quality to be considered.	Science that is not novel, is of unsatisfactory quality, unrealistic objectives, is not timely and is unlikely to advance the field.	The science lacks novelty, is of low quality, not well thought through objectives and is not timely but could result in some useful knowledge.	The proposal is good quality science, which is of very good scientific merit in terms of novelty, quality, objectives, and timeliness and addresses important scientific questions.	The proposal is high quality science, which is of excellent scientific merit in terms of novelty, quality, objectives, and timeliness and addresses highly important scientific questions.	The proposed work meets exceptional scientific standards in terms of novelty, quality, objectives, and timeliness and addresses extremely important scientific questions.
	No Science Case submitted, or at an insufficient quality to be considered.	The research is unlikely to contribute to the understanding of the subject. Not a good match of research to the host group's scientific infrastructure and environment with no benefit to the group and no opportunity to develop new skills.	The research will make a marginal contribution to the understanding of the subject. Not a strong match of research to the host group's scientific infrastructure and environment with little benefit to the group and little opportunity to develop new skills.	The research is not likely to make a significant contribution to the understanding of the subject. Good match of research to the host group's scientific infrastructure and environment with some benefit to the group and the opportunity to develop some new skills .	The research is likely to make a significant contribution to the understanding of the subject. Excellent match of research to the host group's scientific infrastructure and environment with excellent benefit to the group and the opportunity to develop new skills.	The research is highly likely to make a significant contribution to the understanding of the subject. Exceptional match of research to the host group's scientific infrastructure and environment with exceptional benefit to the group and the opportunity to develop new skills.
	No resource requirements/requests or justification submitted, or at an insufficient quality to be considered.	Resource requirements/requests and justification are poorly defined, and cannot be assessed against the guidance criteria.	Resource requirements/requests and justification are not well defined, and cannot accurately be assessed on the guidance criteria.	Resource requirements/requests and justification are defined against the guidance criteria.	Resource requirements/requests and justification are well defined, and can accurately be assessed against the guidance criteria.	Resource requirements/requests and justification are clearly defined against the guidance criteria, and can easily be evaluated.
Management Case	No Project Management or Data Management Case submitted, or at an insuficent quality to be considered.	Plan does not address any of the STFC Project or Data Management frameworks.	Plans covers the minimal percentage the relevant aspects of the Project and Data Management Frameworks outlined by STFC.	Plans cover a large percentage the relevant aspects of the Project and Data Management Frameworks outlined by STFC.	Plans cover all the relevant aspects of the Project and Data Management Frameworks outlined by STFC.	Plans have exceptional coverage of the Project and Data Management frameworks outlined by STFC.
Overall	This research should not be considered	This research should not be supported.	This research should not be supported.	This research could be supported if funds are available.	This research should be supported.	This research programme should definitely be supported and it would be a loss not to do so.

Annex 3: RAC Additional Scoring Considerations

The guidelines for Call 13.5 state that the RAC should take into consideration the additional criteria as follows:

- Alignment of the proposal with the call guidelines.
- Full and effective usage of previous DiRAC allocations.
- Timely submission of interim and final reports of any previous DiRAC allocation.

A score between 0 – 10 will be applied to the RAC additional scoring considerations. This will then form a percentage decrease in the overall score gained from the main criteria with a maximum of 20% decrease in score. For example, a score of 9 would produce a 2% reduction in the final score.

When completing the scoring spreadsheet, RAC members are invited to use this matrix below as a guide for the markings to give for the additional criteria.

Nearer the time, a spreadsheet will be put together to show the usage of previous allocations and the timely submission of interim/final reports. Please refer to this spreadsheet and the scoring matrix below when completing the score sheet.

Score	1-2	3-4	5-6	7-8	9-10
Alignment to call guidelines	Unsatisfactory – deviates from guidelines significantly	Poor – some deviation from guidelines	Good – adheres to guidelines but not fully	Very good – mostly adheres to guidelines	Excellent – matches guidelines exactly
Use of previous allocations	Very poor - little or no usage	Poor usage	Good usage	Very good - used most of allocation	Excellent - used entire allocation
Timely submission of reports	Did not submit	Over 2 weeks late	1-2 weeks late	Less than 1 week late	On time (either in the first instance or after requesting extension)

All three of the criteria should be given equal weight to identify a RAC Additional Score.