

UCL Computational Resource Allocation Group (CRAG)
Monthly Meeting
Wednesday 12th March 2014 at 13.00
Room 104, Podium Building, 1 Eversholt Street, London NW1 2DN

Chair:

1. Prof Nik Kaltsoyannis (NK) – *Molecular Quantum Dynamics and Electronic Structure*

Present:

2. Prof Dario Alfe (DA) – *Thomas Young Centre (Materials Science)*
3. Clare Gryce (CG) – *Head of Research Computing and Facilitation Services, ISD*
4. Ian Kirker (IK) - *Research Comp & Facilitating Services, ISD*
5. Dr Simon Kuhn (SK) – *Engineering Sciences*
6. Dr Andrew Martin (AM) - *Structural & Molecular Biology*
7. Dr Bruno Silva (BCS) – *Research Computing Platforms Team Leader (Service Lead), ISD*
8. Dr Sergey Yurchenko (SY) – *Atomic, Molecular, Optical and Positron Physics*

Apologies:

9. Dr Nicholas Achilleos (NA) – *Astrophysics and Remote Sensing*
10. William Hay (WH) – *Datacentre Services, ISD*
11. Thomas Jones (TJ) – *Research Platforms Team Leader (Infrastructure Lead), ISD*
12. Jo Lampard (JL) - *Senior Research IT Services Facilitator, ISD*
13. Dr Vincent Plagnol (VP) – *Next Generation Sequencing*

In attendance:

14. Corrinne Frazzoni (CF) – *Administrative Services, ISD (Minutes and meeting support)*

Note: Minutes below provide a high level summary of decisions taken and actions assigned by the Group.

1. Approval of Minutes of last meeting held on 14th February 2014

The Group approved the Minutes of the last meeting. There were no matters arising.

2. Update on status of current Actions

The list of current Actions (see table at end) was updated. 6 new Actions were added.

3. Review of any requests for additional resources on local HPC facilities

There were no new requests for additional resources. The previous request from Arash Hamzehloo for exceptional access to run around 200 parallel jobs each with 64 cores for 48 hours was still under discussion. BS suggested discussion to continue via email.

4. Review of Legion usage statistics <http://feynman.rits-isd.ucl.ac.uk:8888>

The month's core availability was still affected by cooling limitations at KLB DC. Only the last week of February 2014 saw an increase in availability. Statistics had been corrected to allow for removal of training accounts. There were 500 accounts of which approximately 300 were dormant. The sudden rise in utilisation and spikes in wait time were as yet unexplained.

Action: Investigate job submission pattern, particularly for Logsdail.

5. Review of IRIDIS and EMERALD usage statistics

The group reviewed the IRIDIS and EMERALD usage statistics for February 2014.

Increased utilisation for both services was resulting in increased job wait times.

Many factors affect wait times, including:

- Institutional consumption of their allocation over the accounting period
- The % share of the HPC service
- Individual consumption of resources
- Job demands
- Other job activity on the system at the time.

Actions: Request breakdown of slowdown per user

Email list of UCL IRIDIS users to advise them that the CRAG is looking at job submission times, noting that there will be extra capacity available from 1 August.

6. Update regarding development of new application form

IK provided a brief update on the new application form.

Action: Functions to add

- **Students to indicate name of PI/supervisor**
- **Add option to change PI/cost centre on system in cases where PI leaves but student remains at UCL.**
- **User to choose from a drop-down menu of research themes (to be defined).**
- **Provide link on form to example of correctly completed form.**
- **Reminders for PIs who have reserved advance resources, when a new user applies**

7. Discussion of the nature and purpose of consortia

The group discussed the nature of the existing research computing consortia and whether or not there was a need for them to continue in their current form for the ongoing management of user accounts and resources. The consortia had originally been founded on an aspiration to support a diverse portfolio of research themes; some had evolved naturally from collaborations.

However, a decision was reached to dissolve the consortia and to replace them with research theme headings (to be defined).

- The leaders of the consortia would be contacted to be advised of the dissolution of the consortia but invited to remain, if they wished, as part of an informal expert advisory community.
- It was agreed that there were some useful things to retain from the current system, such as the ability to assess the appropriateness of a request and the academic oversight of user accounts.
- It was in the interests of the RIISG and UCL to be able to capture data on both the areas of research and the cost centres funding them.
- Users should be able to demonstrate good use of the system, e.g. through reporting on publications and other relevant deliverables.
- Inappropriate requests would be weeded out at application; students and junior researchers would need to provide the name of their supervisor or PI to confirm the request was approved.
- Additional resource requests would need to come from a supervisor or PI.
- The theme headings for accounts would be defined at application via a drop-down list, with possible multiple options for cross-theme research.
- It was agreed to gather a list of research themes, based on those used by funding bodies (e.g. EPSRC) and those used by UCL, to discuss at the next meeting.
- In addition, mailing lists could be set up to associate to the themes, to enable users to contact each other and offer advice and support.
- Further support for new users could be offered by making previously successful applications available to read on the website.

Decision: Dissolve the consortia and replace with research theme headings (to be defined)

**Action: Collate list of research themes. Add as agenda item for April meeting.
Contact the leaders of the dissolved consortia to advise them this will happen and invite to remain as part of an informal expert advisory community.**

8. AOB

There was no other business.

9. Next meeting date and agenda

Friday 4th April 2014 from 13.00-15.00

Venue: Room 104, 1st floor, Podium Building, 1 Eversholt Street, London, NW1 2DN.

Agenda (Items) for the next meeting:

Standing items:

1. Approval of Minutes of last meeting
2. Update on status of current Actions
3. Review of any requests for additional resources on local HPC facilities
4. Review of Legion usage statistics
5. Review of IRIDIS and Emerald usage statistics

New items for next meeting:

- Discussion of research themes.

LIST OF CURRENTLY APPROVED EXCEPTIONAL REQUESTS

Requesting user	CRAG approval date	details of exception	start date agreed	end date agreed	date removed	Implementation Notes
Francesco Lescai	11/10/2013	5 Terabytes of backed up, node-writeable storage. Will implement as 5 terabytes of scratch, with ongoing work to provide backups to NFS-2	1/11/2013	31/03/2014		Currently only a 5TB quota on Scratch is being granted - we have an issue in Github to provide a backup.
Eugenio Pasini	17/01/2014	Scratch quota increased to 1TB for the requested period	17/1/2014	17/4/2014		

LIST OF CURRENT ACTIONS

Shaded (closed/completed) items will be deleted in the next version.

	Actions	Status	Owner
134	KLB Power and Cooling	<p>(12/7/2013): TJ to liaise with Simon Marham for an update regarding KLB's power and cooling upgrade work.</p> <p>(17/9/2013): ONGOING</p> <p>(11/10/2013): ONGOING</p> <p>(22/11/2013): Work currently in progress. ONGOING</p> <p>(13/12/2013): CG chasing up. Group expresses deep concern. ONGOING</p> <p>(17/1/14): If nothing happens by next CRAG then consider escalation to higher governance group. ONGOING</p> <p>(14/2/14): Delayed due to safety issues. ONGOING</p> <p>(12/03/14): Completed. CLOSED</p>	TJ
135	Review of Legion usage statistics	<p>(12/7/2013): BCS to investigate the unexpected wait time spikes for users with small run times.</p>	BCS

		<p>(17/9/2013): ONGOING</p> <p>(11/10/2013): Standing Agenda Item: Identify (full name & user ID) & contact users with systematic problems, try to resolve problems.</p> <p>(22/11/2013): BCS to investigate whether it is possible to remove jobs from the slowdown graph which are part of arrays that have already started.</p> <p>(13/12/2013): Slowdown statistics for job arrays to be calculated according to start time of first job in array only. Check-pointing jobs also to be treated similarly according to initial start time (except for jobs that fail quickly).</p> <p>(17/01/2014): Pending confirmation. ONGOING</p> <p>(14/2/14): ONGOING</p> <p>(12/03/14): Revisit in May – make modifications and review stats from January onwards, comparing to same periods in previous year. ONGOING</p>	
140	General policy proposal for priority access to Research Computing resources	<p>(17/9/2013): BCS to draft new policy to be presented at next meeting.</p> <p>(11/10/2013): ONGOING</p> <p>(22/11/2013): The group would like an explanation of what the value of the 'C' factor included in the leasing calculations is, and how it was derived. NK suggests that the last paragraph belongs before the section about leasing as it relates to buying hardware. Regarding the access policy for purchased and leased nodes, the group would like to see written down some guarantee of how long owners/leasers would have to wait before they could access their nodes. They would also like to see some consideration of the implications for killing active jobs and how this would be handled.</p> <p>(13/12/2013): BCS to recirculate updated priority access document for next meeting including recommendations for two tier pricing system for immediate/delayed access.</p> <p>(17/01/2014): BCS to report back to next CRAG meeting with a proposal for promoting the new policy.</p> <p>(14/2/14): the proposal was made, and will be implemented as follows: Email to the Research Computing Forum Email to the service mailing lists Information to be provided on website in relevant location (TBD) with "promotional" information. ONGOING</p> <p>(12/03/14): CG expressed concern re admin overhead</p>	BCS

		involved in responding to call. Need to be clear on risks and ensure information is out there. Meeting to be held 13/3/14. ONGOING.	
141	Multi-disciplinary research and nature of consortia	<p>(17/9/2013): BCS to provide list of unusual requests for next meeting with Consortia definition and objectives.</p> <p>(11/10/2013): Monitor requests and report to Feb 2014 highlighting any bounced requests by consortia.</p> <p>(22/11/2013): ONGOING</p> <p>(13/12/2013): ONGOING</p> <p>(17/01/2014): ONGOING</p> <p>(14/2/14): Report no monitored requests done, showing a number of cases where applicants had been moved because they misunderstood what the consortia represented. Add discussion to agenda for next meeting. ONGOING</p> <p>(12/03/14): Discussed under item 7. Prepare list of research themes. ONGOING</p>	BCS
145	Web mock-up of new application form	<p>(22/11/2013): Implement changes to form:</p> <ul style="list-style-type: none"> • make data format easier to analyse • look into possibility of populating renewal form with previous year's publications data from RPS • consider back-end support for hosting the form and associated database. <p>(13/12/2013): IK to update form to include information on platforms and produce final version for approval at next meeting.</p> <p>(17/01/2014): The new forms should be implemented subject to the following changes being made:</p> <ul style="list-style-type: none"> - data to be captured on a per project basis - project data only necessary on renewal form if there is a new project - an example of a completed form should be provided to guide users <p>(14/2/14): Covered in Agenda Item 7. New requirements gathered – implementation has started. ONGOING</p> <p>(12/03/14): IK provided update. CLOSED</p>	IK/BCS

146	Create new consortium for Gatsby Centre	<p>(22/11/2013): Make the necessary arrangements and changes to set up the Gatsby Centre consortium.</p> <p>(13/12/2013): ONGOING</p> <p>Consortium to be added pending new application process implementation</p> <p>(17/01/2014): ONGOING</p> <p>(14/2/14): ONGOING</p> <p>(12/03/14): CLOSED</p>	BCS
150	Statistical science legion access query	<p>(17/01/2014): BCS to advise statistical science of the CRAG's view that the standard access policy should be followed for centrally funded resources but that a departmental reserve may have its own policy.</p> <p>(14/2/14): Document to send to Stats department is being finalised. ONGOING</p> <p>(12/03/14): BS sent document to stats dept; awaiting feedback. CLOSED</p>	BCS
151	KPI for legion wait times	<p>(17/01/2014): After correcting for job arrays, mean slowdown will be calculated for each job type (single core, single node, multi-node etc.) on a monthly basis. The use of this measure will be evaluated at a subsequent CRAG meeting.</p> <p>(14/2/14): This is now being done for senior management reports – will be introduced in coming Legion statistics reports. ONGOING</p> <p>(12/03/14): ONGOING</p>	BCS
152	Job submission patterns	<p>(12/03/14): Investigate job submission pattern, particularly for Logsdail. NEW ACTION</p>	BCS
153	Slowdown	<p>(12/03/14): Request breakdown of slowdown per user. NEW ACTION</p>	BCS
154	Job submission times	<p>(12/03/14): Email list of UCL IRIDIS users to advise that CRAG looking at job submission times, noting there will be extra capacity available from 1 August. NEW ACTION</p>	BCS

155	Functions to add to application system	<p>(12/03/14): Functions to add to application system</p> <ul style="list-style-type: none"> - Students to indicate name of PI/supervisor - Add option to change PI/cost centre on system in cases where PI leaves but student remains at UCL. - User to choose from a drop-down menu of research themes (to be defined). - Provide link on form to example of correctly completed form. - Reminders for PIs who have reserved advance resources, when a new user applies <p>NEW ACTION</p>	IK
155	Research themes for user accounts	<p>(12/03/14): Collate list of research themes, based on those used by funding bodies e.g. EPSRC and those used by UCL. Add to April agenda. NEW ACTION</p>	BCS/CF
156	Dissolution of consortia	<p>(12/03014): Contact the leaders of the dissolved consortia to advise them of this and invite to remain as part of an informal expert advisory community. NEW ACTION</p>	BCS