

# UCL Computational Resource Allocation Group (CRAG)

## MEETING MINUTES

12<sup>th</sup> July 2013

### In Attendance:

1. Prof Nik Kaltsoyannis (Chair) - *Molecular Quantum Dynamics and Electronic Structure*
2. Dr Ben Waugh - *High Energy Physics*
3. Dr Bruno Silva - *Research Computing Platforms Team Leader (Service Lead), ISD*
4. Jo Lampard - *Senior Research IT Services Facilitator, ISD*
5. Tom Couch - *Senior Research IT Services Facilitator, ISD*
6. Dr Vincent Plagnol – *Next Generation Sequencing*
7. Thomas Jones - *Research Platforms Team Leader (Infrastructure Lead), ISD*

### Apologies:

1. Dr Andrew Martin - *Bioinformatics and Computational Biology*
2. Dr Nicholas Achilleos - *Astrophysics and Remote Sensing*
3. Clare Gryce - *Head of Research Computing and Facilitating Services, ISD*
4. Prof Dario Alfe - *Thomas Young Centre (Materials Science)*

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

### **1. Approval of Minutes of last meeting on 14<sup>th</sup> June 2013**

The Group approved the Minutes of the June 14<sup>th</sup> 2013 meeting, pending amendments.

### **2. Update on status of current Actions**

The list of current Actions (below) was updated, and new Actions arising were added.

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

There were none for the current month.

#### 4. Review of any Centre for Innovation (Cfi) access requests (Chair)

The following applications were approved:

- IRIDIS: Abhishek Kumar Mishra
- EMERALD: Bradley Treeby
- EMERALD: Hans Koss

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

BCS presented the Legion statistics for June 2013, and explained that the number of available nodes had decreased due to power and cooling limitations at the KLB datacentre and an outage caused by an authentication subsystem failure that affected MPI jobs only.

The KLB problems can be resolved by upgrading the power and cooling at the KLB data centre. TJ to liaise with Simon Marham for an update on this work (**see new action 134**).

Service availability was at 100%. It was thought there were unexpected spikes in wait time for users with very small CPU utilisation. BCS to investigate this (**see new action 135**).

#### 6. Review of IRIDIS and EMERALD usage statistics

*(Doc: Cfi stats June.pptx)*

BCS presented the Cfi service utilisation statistics for EMERALD and IRIDIS. NK was concerned that EMERALD utilisation was lower again and it was imperative to increase EMERALD awareness across UCL. VP enquired as to whether users from the Francis Crick Institute could have access to EMERALD. BCS informed all that EMERALD offered 8% for external access, however if Francis Crick Institute was collaborating with UCL partners then UCL visitors access would be granted for EMERALD via the normal application process.

It was noted that UCL had increased its uptake to IRIDIS.

BCS to confirm whether UCL has now ½ of total IRIDIS allocation available to researchers (**see new action 136**).

#### 7. General policy proposal for priority access to Research Computing resources (Clare Gryce)

This item to be discussed at next meeting

#### 8. General policy and process proposal for access to Research Computing resources (Bruno Silva)

BCS presented a proposal draft for a single access request form to UCL-based research platforms as well as Cfi platforms. As per the current process, the consortium leaders would do a very light-weight peer review of each application made for their consortium. For Cfi platform access, the user would be required to give a justification for their request which would also be reviewed by the consortium

leaders from a scientific point of view and by the RC team from a technical point of view. NK stated that Cfi applications are more difficult and should be reviewed by the CRAG for discussion and decision. BCS suggested that access to applications for Cfi be placed into a separate repository which then could be reviewed by the CRAG. It was decided that the following headings also be added to the application form to comply with the information currently being requested to comply with Cfi objectives:

- Project Objective/Abstract
- Technical Abstract

It was decided that BCS should bring a mock-up of the application form for the next meeting.

**(see new action 137).**

## **9. AOB**

It was highlighted that a number of requests of accounts between consortia was increasing and perhaps this indicated that users did not know whether they should apply for consortia based on either a science or technical aspect. NK indicated that consortia applications should always be made based on technical aspect.

Exceptions on Legion to be added to the CRAG minutes and reviewed on a monthly basis **(see new action 138).**

## **10. Next Meeting Date and Agenda**

9<sup>th</sup> August 2013 from 1pm – 3pm, Cruciform Foyer 102 Seminar Room 2, Cruciform Building, GOWER STREET, LONDON, WC1E 6BT

### **Agenda (Items) for the next meeting:**

General policy proposal for priority access to Research Computing resources (Clare Gryce)

### **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 any Centre for Innovation (Cfi) access requests (Chair)
5. Review of Legion usage statistics,
6. Review of IRIDIS and Emerald usage statistics

### **New item:**

- 1 General process for Priority access

## LIST OF CURRENT ACTIONS

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

	<b>Actions</b>	<b>Status</b>	<b>Owner</b>
96	Record of Cfl applications	<p>(9/11/2012): It was agreed that a spreadsheet record of all Cfl requests, including reasons for rejection where appropriate, should be maintained.</p> <p>11/1/2013 – CG to maintain list of usage and report to CRAG every three months.</p> <p>(8/2/2013): ONGOING – update next month</p> <p>(15/3/2013): ONGOING</p> <p>(19/4/2013): CG has set up the spread sheet with BCS to maintain.</p> <p>(10/5/2013): CG to hand over to BCS.</p> <p>(14/6/2013): ONGOING</p> <p><b>(12/7/2013): ONGOING</b></p>	BCS
110	Consortia mailing list	<p>(11/1/2013): BCS to advertise Consortia mailing lists on the Research Computing webpage with an archive and search facility for consortium members.</p> <p>(8/2/2013): The archives are not searchable at the moment; TJ to request that the lists are transferred to Mailman which will allow this. It may not be possible to have a single cross-searchable archive for all the lists. TJ will find out if non-members can have read-only access. BCS will add links for each archive to the web pages if necessary.</p> <p>(8/2/2013): BS to replace/update mailing list on consortia webpage and send mailman links to consortia leaders to view all messages.</p> <p>(15/03/2013): Mailman mailing lists added to consortia webpage. Mailman mailing list links not sent yet.</p> <p>(19/4/2013): Consortium leaders still need to be sent information about their respective mailing lists; TJ to do this.</p> <p>(10/5/2013): TJ reported problems/issues re mailing lists to mailing team.</p> <p>(14/6/2013): ONGOING</p> <p><b>CLOSED</b></p>	TJ and BCS

114	Legion scratch quotas	<p>(8/2/2013): BCS to implement increased Legion scratch quotas of double the existing default allocation (200Gb).</p> <p>(15/03/2013): ONGOING</p> <p>(19/04/2013): The recent issue with NFS over the preceding weekend had prevented TJ from switching scratch quotas back on; the information has been updated, but the database needs to be moved to another server in case that was the cause of the problem. Once done, TJ will be implementing the increase to 200Gb default allocation next week.</p> <p>(10/5/2013): To go live 14.05.2013</p> <p>(14/6/2013): ONGOING</p> <p><b>CLOSED</b></p>	BCS/TJ
115	<p>Amend stats graph so that zero-utilising Consortia are still shown. Legion usage Report available</p> <p><a href="http://feynman.rits-isd.ucl.ac.uk:8888">http://feynman.rits-isd.ucl.ac.uk:8888</a></p>	<p>(15/3/2013): BS to present graph of slowdown per user using both requested time and run time.</p> <p>(19/04/2013): ONGOING</p> <p>(10/5/2013): ONGOING</p> <p>(14/6/2013): ONGOING</p> <p><b>(12/7/2013): Zero graphs pending</b></p>	BCS
117	Dr. Oleg L. Polyansky	<p>(15/03/2013): BCS to liaise with Oleg L. Polyansky to establish limit for backfill pending further steer on IRIDIS access from Cfl Research Policy group.</p> <p>(19/04/2013): BCS has spoken to Oleg and his colleague Lorenzo; the backfill limit has been removed as there is a large variance in runtime. To be reviewed after one month.</p> <p>(10/5/2013): BCS to contact Oleg regarding access to IRIDIS, to also acquire usage requirement statistics and details of total amount of resource required. In order for RC to identify approximately the number of jobs to be submitted by Oleg. To be reviewed after one month.</p> <p>(14/6/2013): ONGOING</p> <p><b>(12/7/2013): Continue with special consideration for HPC work.</b></p>	BCS
119	<p>Legion usage Report available</p> <p><a href="http://feynman.rits-isd.ucl.ac.uk:8888">http://feynman.rits-isd.ucl.ac.uk:8888</a></p>	<p>(15/3/2013): BS to present graph of slowdown per user using both requested time and run time.</p> <p>(19/04/2013): ONGOING</p> <p>(10/5/2013): ONGOING</p>	BCS

		(14/6/2013): ONGOING <b>CLOSE</b>	
122	John Brodholt – IRIDIS application	(19/04/2013): BCS to inform John that his Leeds collaborators will be required to apply for UCL usernames before the application can be approved. CG to investigate the possibility of the IRIDIS job scheduler automatically diverting jobs only requiring a small number of cores to the low quality service partition.  (10/5/2013): ONGOING (14/6/2013): ONGOING <b>CLOSED</b>	BCS/CG
124	Legion usage - job wait time anomalies	(19/04/2013): BCS to investigate the very short wait times for the TYC consortium, and the long wait times for users uccajab and zccamku.  (10/5/2013): BCS to contact uccajab and zccamku to establish and understand their jobs, perhaps suggest compacting jobs.  (14/6/2013): ONGOING <b>CLOSED</b>	BCS
125	Increasing Emerald support and awareness	(19/04/2013): CG to contact Istvan Reguly (to arrange a visit to VP's group).  An email to be sent out an email to Legion users highlighting the applications already installed on Emerald and offering pre-booked desktop support visits.  The possibility of holding a one-day CUDA Workshop GPU event to be discussed.  (10/5/2013): Handed over to JL to circulate email, organise a CUDA (GPU) workshop for UCL Genetics Institute (VP) as well as organise further GPU workshops for UCL depts.  (14/6/2013): ONGOING <b>CLOSED</b>	JL
126	New Legion/IRIDIS access policy	(19/04/2013): The Research Computing team to produce a new draft access policy and bring to the next meeting for discussion/approval. A single account application form for Legion and IRIDIS to be designed. The possibility of automatic IRIDIS account creation for existing Legion users to be investigated. Exceptional IRIDIS users to be migrated to the high quality service partition to be identified as soon as	CG/BCS

	Cfl Proposal for Acces to Facilities application form	<p>possible.</p> <p>(10/5/2013): ONGOING</p> <p>(14/6/2013): ONGOING</p> <p><b>(12/7/2013): ONGOING</b></p> <p>(10/5/2013): BCS to re-design the Cfl Proposal for Access to Facilities application form for review by July.</p> <p>(14/6/2013): Review project abstract section to allow general reading.</p> <p><b>(12/7/2013): Proposal presented. BCS bring a mock-up of application form for access UCL research platforms</b></p>	BCS
131	IRIDIS and EMERALD usage statistic	<p>(14/6/2013): BCS to liaise directly with Derek Cross and Timothy Metcalf to seek further clarification on statistics presented for EMERALD</p> <p><b>(12/7/2013): ONGOING</b></p>	BCS
132	Legion users to migrate to IRIDIS	<p>(14/6/2013): Legion users, as those with the highest core count would be migrated to IRIDIS. It was agreed that BCS would identify and provide a list of users of 32 cores and above.</p> <p><b>(12/7/2013): BCS has created list and will initiate IRIDIS accounts and migrate (with overlap period of 3 months) users accordingly. List to be presented at next meeting.</b></p>	BCS
133	IRIDIS expansion budget	<p>(14/6/2013): CG to provide update after one month.</p> <p><b>(12/7/2013): ONGOING</b></p>	CG
134	KLB Power and Cooling	<p><b>(12/7/2013): TJ to liaise with Simon Marham for an update regarding KLB's power and cooling upgrade work.</b></p>	TJ
135	Review of Legion usage statistics (June)	<p><b>(12/7/2013): BCS to investigate the unexpected wait time spikes for users with small run times.</b></p>	BCS
136	UCL IRIDIS access	<p><b>(12/7/2013): BCS to confirm, UCL have full allocation of nearly 6000 cores on IRIDIS.</b></p>	BCS
137	Mock-up web base application form	<p><b>(12/7/2013): BCS to bring a mock of web base application form to the next meeting..</b></p>	BCS

138	Exceptions on Research computing platforms.	<b>(12/7/2013): BCS to produce list of current exceptional request to be reviewed by CRAG.</b>	BCS
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