

UCL Computational Resource Allocation Group (CRAG)

MEETING MINUTES

14th June 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. Clare Gryce - *Head of Research Computing and Facilitating Services, ISD*
5. Jo Lampard - *Senior Research IT Services Facilitator, ISD*
6. Tom Couch - *Senior Research IT Services Facilitator, ISD*
7. Prof Dario Alfe - *Thomas Young Centre (Materials Science)*

Apologies:

1. Dr Andrew Martin - *Bioinformatics and Computational Biology*
2. Dr Nicholas Achilleos - *Astrophysics and Remote Sensing*
3. Dr Vincent Plagnol – *Next Generation Sequencing*
4. Thomas Jones - *Research Platforms Team Leader (Infrastructure Lead), ISD*

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 10th May 2013

The Group approved the Minutes of the May 10th 2013 meeting.

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

The following applications were approved:

- IRIDIS: Anna Gould
- EMERALD: Thomas Collier
- EMERALD: Mark Williams
- EMERALD: Ming Ma

The following application was approved pending further information:

- EMERALD: Francesco Carbone

It was agreed that feedback be given to Francesco Carbone to present further detailed information in the project abstract section of the application form. It was also agreed that the Centre for Innovation – Proposal for Access to Facilities form be reviewed and that the project abstract section be revised to allow for general reading.

(see new Action 130).

5. Review of IRIDIS and EMERALD usage statistics

(Doc: Cfi May 2013 stats.pdf)

CG presented the Cfi service utilisation statistics for EMERALD and IRIDIS. NK stipulated that UCL had been allocated 25% usage of EMERALD. BCS was concerned that various statistics and nodes had not been reflected in CPU utilisation. BCS to liaise directly with Derek Cross and Timothy Metcalf to seek further clarification on statistics presented for EMERALD

(see new Action 131).

It was reported that the uptake for IRIDIS had increased and that the UCL 50% allocation seemed to have been utilised. CG gave an update on the IRIDIS expansion, UCL allocation had been set at 6,000 cores however this really equated to 11,800 cores. UCL had been allocated access to expanded IRIDIS for one year.

It was suggested that an alternative priority access implementation could be to give high priority to 32 core jobs and above, where 32 cores really equated to 36 cores. Once this was implemented, CRAG would then review the statistics after three months. NK enquired whether this would have any implication on moving users from Legion, NK was informed that there would be no implication upon 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.
(see new Action 132).

CG also informed all that UCL had budget in place to fund 50% ongoing access at current level for IRIDIS. CG to update all, after one month.
(see new Action 133).

6. AOB

None

7. Next Meeting Date and Agenda

12th July 2013 from 1pm – 3pm, Cruciform Foyer 102 Seminar Room 2, Cruciform + Building, GOWER STREET, LONDON, WC1E 6BT

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 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 Prioritisation for Priority access

LIST OF CURRENT ACTIONS

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

	Actions	Status	Owner
91	Establish policy for requesting Priority CP hours	<p>(10/09/2012): CG to circulate draft policy paper to CRAG members and inform Serge Guillas that his request is under review. All CRAG members to report back on implementation of Priority Queue.</p> <p>(12/10/2012): TJ to investigate implementation of Priority Access using 'Projects' method as discussed and agreed by group. Gold Accounting Software – RC to investigate by further testing. NA to provide local Miracle users for testing.</p> <p>(9/11/2012): Still pending. Meanwhile, TJ to set up priority access for Miracle jobs as previously agreed using same set up on Miracle as for Harvest project (Serge Guillas).</p> <p>(14/12/2012): Done for Miracle jobs; TJ to present Gold accounting software information at the next CRAG.</p> <p>(14/12/2012): Gold accounting software installed. Client and lustre upgrade still pending. TJ to report back at next CRAG.</p> <p>(8/2/2013): TJs team are testing, looking into SGE and thinking about how to implement it. TJ to write up and report at next CRAG.</p> <p>(15/3/2013): Gold accounting software installed, configured and deployed on 18/3/2013.</p> <p>(19/4/2013): Agenda item for the next meeting to review and approve the draft policy for access to the Priority Queue.</p> <p>CLOSED</p>	TJ
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>	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>	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>	BCS/TJ
115	Amend stats graph so that zero-utilising Consortia are still shown. Legion usage Report available http://feynman.rits-isd.ucl.ac.uk:8888	<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>	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>	BCS
119	Legion usage Report available http://feynman.rits-isd.ucl.ac.uk:8888	<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>	BCS
121	Michail Stamatakis UCL Chemical Engineering, £35k funding for computing infrastructure	<p>(15/3/2013): BS to report back to CRAG on:</p> <ul style="list-style-type: none"> • Costing • Integration • Hosting <p>(19/04/2013) BCS has obtained hardware costings as part of the process for the next upgrade and is to meet with Michail in the next few days. TJ also needs to get costings for hosting. They have not yet agreed on whether there will be a common software stack.</p> <p>(10/5/2013): CG to obtain true operational cost i.e. overheads, data resources which must be passed on. To note that this is not offered as a service but as a pilot project. To be reviewed in one month.</p> <p>(10/5/2013): BCS to inform Michail Stamatakis of three minimum priority access time.</p> <p>CLOSED</p>	BCS
122	John Brodholt – IRIDIS application	<p>(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</p>	BCS/CG

		<p>low quality service partition.</p> <p>(10/5/2013): ONGOING</p> <p>(14/6/2013): ONGOING</p>	
123	Kristen Marino – IRIDIS application	<p>(19/04/2013): BCS to speak to Kristen to see if her GROMACS jobs are suitable for running on Emerald.</p> <p>(10/5/2013): BCS to contact Kristen and establish if her GROMACS jobs are successfully running on EMERALD, also suggest that Kristen contact GPU specialist at Cfl.</p> <p>CLOSED</p>	BCS
124	Legion usage - job wait time anomalies	<p>(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.</p> <p>(10/5/2013): BCS to contact uccajab and zccamku to establish and understand their jobs, perhaps suggest compacting jobs.</p> <p>(14/6/2013): ONGOING</p>	BCS
125	Increasing Emerald support and awareness	<p>(19/04/2013): CG to contact Istvan Reguly (to arrange a visit to VP's group.</p> <p>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.</p> <p>The possibility of holding a one-day CUDA Workshop GPU event to be discussed.</p> <p>(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.</p> <p>(14/6/2013): ONGOING</p>	JL
126	New Legion/IRIDIS access policy	<p>(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 possible.</p> <p>(10/5/2013): ONGOING</p> <p>(14/6/2013): ONGOING</p>	CG/BCS

127	David Wright IRIDIS application	(10/5/2013): BCS to investigate why this application is not suitable for EMERALD. CLOSED	BCS
128	Cfl Proposal for Acces to Facilities application form	(10/5/2013): BCS to re-design the Cfl Proposal for Access to Facilities application form for review by July.	BCS
129	Legion Priority Queue access costing	(10/5/2013): BCS and TJ to liaise with Miracle and HECToR teams to understand how they cost priority access. CLOSED	BCS/TJ
130	Centre for Innovation – Proposal for Access to Facilities form	(14/6/2013): Review Centre for Innovation – Proposal for Access to Facilities form and review project abstract section to allow general reading.	BCS
131	IRIDIS and EMERALD usage statistic	(14/6/2013): BCS to liaise directly with Derek Cross and Timothy Metcalf to seek further clarification on statistics presented for EMERALD	BCS
132	Legion users to migrate to IRIDIS	(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.	BCS
133	IRIDIS expansion budget	(14/6/2013): CG to provide update after one month.	CG