

UCL Computational Resource Allocation Group (CRAG)

MEETING MINUTES

17th September 2013

In Attendance:

1. Prof Nik Kaltsoyannis (Chair) - *Molecular Quantum Dynamics and Electronic Structure*
2. Dr Bruno Silva - *Research Computing Platforms Team Leader (Service Lead), ISD*
3. Jo Lampard - *Senior Research IT Services Facilitator, ISD*
4. Tom Couch - *Senior Research IT Services Facilitator, ISD*
5. Dr Andrew Martin - *Bioinformatics and Computational Biology*
6. Dr Nicholas Achilleos - *Astrophysics and Remote Sensing*
7. Prof Dario Alfe - *Thomas Young Centre (Materials Science)*
8. Thomas Jones - *Research Platforms Team Leader (Infrastructure Lead), ISD*
9. Prof Eric Fraga – *Engineering Sciences, Optimisation, Data Analysis and Molecular Dynamics*

Apologies:

1. Dr Ben Waugh - *High Energy Physics*
2. Dr Vincent Plagnol – *Next Generation Sequencing*
3. Clare Gryce - *Head of Research Computing and Facilitating Services, 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 12th July 2013

The Group approved the Minutes of the June 12th 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

The following applications were approved:

- UNITY: Yasmine Al Hamdari

BCS commented, that Enrico Berado had been informed that the request for additional resource on IRIDIS had not been possible. However, Enrico Berado could use the High Memory nodes on Legion which could be requested via the Legion Scheduler.

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

The chair informed all that the current process for EMERALD would remain, however high priority exceptional requests based on volume would be reviewed by the CRAG.

The following applications were approved:

- IRIDIS: David Santos-Carballal

The application for additional resource on IRIDIS from Michail Stamatakis was denied as IRIDIS would not be useful for his jobs. BCS to contact Michail Stamatakis and offer priority use of Legion. BCS to establish how long the job will take.
(see new action 139)

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

BCS presented the Legion statistics for July and August 2013, DA commented that July statistics suggested an anti correlation between wait time and CPU time and that single core jobs were successful on any cluster as the cluster was more utilised. BCS informed all that many jobs did not go through in August 2013 due to Data Centre issues and that new nodes of 16 cores and 64GB RAM had been added to the cluster on 20th August 2013. Users were to be informed at the end of September 2013 that High Memory nodes would be available on Legion. NA enquired if GPU training would be available to enable users to utilise the additional computing power offered presently in GPU nodes on Legion and EMERALD. JL informed all that GPU training workshops had been organized and that RC would continuing offering information about third party courses when available.

6. Review of IRIDIS and EMERALD usage statistics

BCS presented the Cfi service utilisation statistics for EMERALD and IRIDIS. It was noted that UCL usage of IRIDIS was stable and August Statistics indicated a high external use of EMERALD.

7. General policy proposal for priority access to Research Computing resources (Bruno Silva)

(Doc: Legion priority access policy (Bruno).docx)

It was agreed that the current Legion priority access policy was out dated and required revising. NK suggested the new draft policy contain two options as follows:

- 1) Hardware purchase to augment Legion (buy kit)
- 2) Special Resource Allocation

NK requested that it was imperative to have information pertaining to monetary cost and the cost of impact on users, as well as governance with regards to option 1. BCS informed all, of the current working example of Dr Michail Stamatakis from the department of Chemical Engineering, whereby the Department purchased 8 nodes of 64 cores for infiniband. The purchasing of hardware allowed backfill when the hardware was not used by the purchaser. AM suggested a simple equipment leasing policy e.g 10% of resource and monthly cost of CPU multiplied by 32 and then doubled. It was agreed that the leasing of existing resource would be reviewed by the CRAG, only if and when the situation arose. New draft policy to be presented at next meeting.

(see new action 140)

8. Update on migration of users to IRIDIS with jobs greater than 36 cores (Bruno Silva)

Bruno Silva to inform Legion users that IRIDIS will be available to those requiring 36 cores or more on Legion.

(see action 132)

9. Very large job policy (<1000nodes) on IRIDIS – should scaling tests be required? (Bruno Silva)

BCS informed all that a request had been undertaken for the use of the whole of IRIDIS which subsequently failed. BCS informed all that there were no Cfi procedures or governance in place for such requests. NK indicated that if UCL users wished to use UCLs allocation on IRIDIS (6,000 cores), such a request would need to be made to the CRAG for analysis. And that until the whole of Cfi agreed mutual governance and procedures, UCL users would be limited to 100 nodes (Southampton set limit) and no scaling tests would be undertaken.

10. Multi-disciplinary research and nature of consortia (Bruno Silva)

BCS informed all that UCL consortia seemed to be getting increased amounts of unusual requests that did not fit in the current consortia list. It was agreed that a list of unusual requests be provided at the next meeting, with consortia definition and objectives and to review whether the current list of consortia reflect UCLs actual computational research.

(see new action 141).

11. Next Meeting Date and Agenda

11th October 2013 from 1pm – 3pm, Venue: Podium Building, 1 Eversholt Street, London, NW1 2DN.

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 and policy for Priority access + Leasing of existing HPC resources

Active special requests:

Requesting user(s)	set up by	CRAG approval date	details of exception	start date agreed	end date agreed
Winston Lau Nicolas Maniatis	Ian Kirker	20/12/2012	7-day queue (GPU nodes) on Legion		
John Buckeridge	Owain Kenway	28/05/2012	7-day queue for VASP jobs		
Isaac Sugden	Brian Alston	11/01/2013?	7/10 day unity queue		
Alison Wright	Bruno Silva	15/03/2013	10 day wall clock time limit on Unity	25/03/2013	25/06/2013 (review at this time)
Oleg Polyansky	requested CFI IRIDIS account and was given full wall clock time allowance for backfill on Legion (he is currently running 30 hour jobs)	15/03/2013	backfill limit on nodes of type W lifted to 48 hours	12/04/2013	11/09/2013
Enrico Berardo	Owain Kenway	18/09/2013	would like to run 2 different jobs occupying 96 cores for 144 hours		
Yasmine	Owain Kenway	18/09/2013	Extended time of 14 days per job for a total of four 32 core jobs Unity.		

LIST OF CURRENT ACTIONS

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

	Actions	Status	Owner
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>(12/7/2013): ONGOING</p> <p>CLOSED</p>	BCS
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> <p>(12/7/2013): ONGOING</p> <p>(17/9/2013): Zero graphs pending</p>	BCS
117	Dr. Oleg L. Polyansky (Keep this item open until a significant number of people move to IRIDIS)	<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>	BCS

		<p>(14/6/2013): ONGOING</p> <p>(12/7/2013): Continue with special consideration for HPC work.</p> <p>(17/9/2013): Continue with special consideration for HPC work.</p>	
126	<p>New Legion/IRIDIS access policy</p> <p>Cfl Proposal for Acces to Facilities application form</p>	<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> <p>(12/7/2013): ONGOING</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>(12/7/2013): Proposal presented. BCS bring a mock-up of application form for access UCL research platforms.</p> <p>(17/9/2013): CLOSED</p>	<p>CG/BCS</p> <p>BCS</p>
131	<p>IRIDIS and EMERALD usage statistic</p>	<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>(12/7/2013): ONGOING</p> <p>(17/9/2013): ONGOING</p>	BCS
132	<p>Legion users to migrate to IRIDIS</p>	<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>(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.</p> <p>(17/9/2013): BCS to inform users of migration decision and of policy, and to contact individual users (using</p>	BCS

		cores greater than 36.	
133	IRIDIS expansion budget to fund 50% on-going access at current level for IRIDIS	(14/6/2013): CG to provide update after one month. (12/7/2013): ONGOING (17/9/2013): CLOSED	CG
134	KLB Power and Cooling	(12/7/2013): TJ to liaise with Simon Marham for an update regarding KLB's power and cooling upgrade work. (17/9/2013): ONGOING	TJ
135	Review of Legion usage statistics	(12/7/2013): BCS to investigate the unexpected wait time spikes for users with small run times. (17/9/2013): ONGOING	BCS
136	UCL IRIDIS access	(12/7/2013): BCS to confirm, UCL have full allocation of nearly 6000 cores on IRIDIS. (17/9/2013): CLOSED	BCS
137	Mock-up web base application form	(12/7/2013): BCS to bring a mock of web base application form to the next meeting. (17/9/2013): ONGOING	BCS
138	Exceptions on Research computing platforms.	(12/7/2013): BCS to produce list of current exceptional requests to be reviewed by CRAG. (17/9/2013): ONGOING	BCS
139	Additional Resource request: IRIDIS	(17/9/2013): BCS will contact Michail Stamatakis, and offer priority use of Legion and establish how long his jobs will take.	BCS
140	General policy proposal for priority access to Research Computing resources	(17/9/2013): BCS to draft new policy to be presented at next meeting.	BCS

141	Multi-disciplinary research and nature of consortia	(17/9/2013): BCS to provide list of unusual requests for next meeting with Consortia definition and objectives in	BCS
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