

UCL Computational Resource Allocation Group (CRAG)

MEETING MINUTES

12th October 2012

In Attendance:

1. Clare Gryce (Chair) - *Head of Research Computing and Facilitating Services, ISD*
2. Prof Dario Alfe - *Thomas Young Centre (Materials Science)*
3. Dr Nicholas Achilleos - *Astrophysics and Remote Sensing*
4. Dr Vincent Plagnol – *Next Generation Sequencing*
5. Thomas Jones - *Research Platforms Team Leader (Infrastructure Lead), ISD*

Apologies:

1. Prof Andrew Philips - *Epidemiology*
2. Dr Andrew Martin – *Bioinformatics and Computational Biology*
3. Prof Nik Kaltsoyannis (Chair) - *Molecular Quantum Dynamics and Electronic Structure*
4. Dr Bruno Silva - *Research Computing Platforms Team Leader (Service Lead), ISD*
5. Dr Ben Waugh – *High Energy Physics*
6. Dr Dugan Witherick - *Astrophysics and Remote Sensing*

Note: Minutes below provide a high level summary of decisions taken and actions assigned by the Group. CRAG members are referred to the slide deck for the meeting for further information on matters presented.

1. Approval of Minutes of last meeting on 10th September 2012

The Group did not approve the Minutes of the September 10th 2012. CG to approve minutes, pending off-line amendments.

2. Update on status of current Actions

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

3. Any requests for additional resources: (a) scratch quota requests, (b) any other request.

Scratch Quota requests

The following requests were approved:

Professor Eric S Fraga, Santos Chair of Energy & Resources, Academic Director, School of Energy and Resources, UCL Australia – it was agreed that Prof Fraga should be advised that extended quote may be subject to review by the CRAG at any time as associated policy evolves.

Any other requests:

None

4. Review of Legion usage stats using new online reporting framework (Bruno Silva)

CG gave a brief explanation of Legion usage stats.

5. Update on proposal for Centre for Innovation access policy (Clare Gryce), document: *Cfl_Access_Applications_v0.5*

CG explained that the scope of this policy and document was to offer flexibility and optimisation of HPC usage across all platforms available to UCL researchers, placing responsibility on the researcher to explain why a particular calculation or workload may be more appropriately performed on Emerald, thus also minimising the administrative overhead for the CRAG. CG stressed that as usage of the Cfl facilities increased then the CRAG may need to review and become more selective. Once policy and draft application document have been approved by CRAG and Research Computing Working Group, CG proposed the following:

- Cfl usage is incorporated into CRAG reports.
- Access policy launch on website
- Present and review all applications at CRAG meetings

The policy and document was approved as a working document to monitor applications. Both policy and document to be launched end of October 2012, and the first cohort of applications to be reviewed December 2012.

6. Verbal update on Legion IV project (*Clare Gryce on behalf of Bruno Silva*)

Clare Gryce gave the following update:

- Synthetic testing of metadata performance of file stores is now complete.
- User workload testing on new file system, to take place 13th October 2012.

- Old directory structure has been replicated on to new structure resulting in faster service.
- Next phase of the project will be an expansion of compute capacity, with approach to be approved by Research Computing Working Group.

7. Next Meeting Date and Agenda

- 9th November 2012 from 1pm – 3pm, Room B3A South Wing, Main UCL Building, Cruciform Building, Gower Street London, WC1E 6BT.

Agenda Items:

- 1 Longevity of Legion user accounts added or renewed.
- 2 What to do regarding:
 - 7-day jobs (Gaussian)
 - Privileged Users benefiting from these 7-day
- 3 What do we want from Consortia leaders? (*WG 1 meeting of 16.10.12*)
- 4 Which Data should be allowed to users? (*WG 1 meeting of 16.10.12*)
- 5 To provide data regarding use of Legion by taught students (*27.4.12 – ownership changed to NK as new Chair of CRAG*).
- 6 Need for policy regarding use of Legion by taught students (*Agreed WG 1 meeting of 16.10.12*)

LIST OF CURRENT ACTIONS

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

	Actions	Status	Owner
73	Devise proactive strategy to inform users of the availability of Condor.	<p>(25.11.11): Email consortium leaders and speak to members of the Genomics community (Jacky Pallas perhaps) regarding Condor to move this forward.</p> <p>(27/01/2012): Pending completion of on-going works to improve usability of Condor service.</p> <p>(24/02/2012): IN PROGRESS. Usability works still in progress; OK to liaise with ISD Datacentre Services to create shared storage for users to install applications (e.g. R & Python) via Research Computing.</p> <p>(30/03/2012): IN PROGRESS. Technical issues regarding mounting of shared storage currently undergoing testing.</p> <p>(24/05/2012): IN PROGRESS. Technical issues regarding mounting of shared storage currently undergoing testing</p> <p>(26/06/2012): IN PROGRESS. Shared storage areas have been mounted on Condor machines, applications require placement.</p> <p>(25/07/12): Can now mount and start moving users. Going to make Condor useable from Legion itself, and should be available by next year. Will be a hybrid system.</p> <p>(10/09/2012): Modification to Condor successful. Users will be contacted to move their web jobs for Condor.</p> <p>(12/10/2012): We have found unexpected problems mounting the K drive – we are investigating what the problem is. Nevertheless, condor is usable.</p>	BCS
76	Peter Harrison request for additional Unity resource	<p>(27/01/2012): To follow up with requestors regarding additional information about check-pointing and problem decomposition.</p> <p>(24/02/2012): Update from DG, Peter Harrison has been working closely with RC team and adapting code where possible. CRAG agreed to extend 72hr wall-clock to 10 days on Unity. CLOSED to be REVISTED at a later date</p> <p>(24/05/2012): DG to contact the user regarding progress of his work.</p> <p>(26/06/2012): Re-assigned to BCS</p> <p>(25/07/2012): BCS to speak to contact Peter Harrison.</p>	BCS

		(10/09/2012): PH requests continued use of Unity and will provide review for next CRAG meeting. (12/10/2012): CRAG approved Peter Harrison's indefinite request with proviso that Legion is cited in research papers. BCS to provide update to CRAG in 3 months.	
87	Reports on key publication reports to be used for promoting Legion	(24/4/2012 – Action opened: NK to email Consortium Leaders asking them to solicit lists of key publications that have been enabled via use of Legion, for use on RC website and to encourage more requests for additional resources. (26/6/2012): Link publications on RC website and provide list of Consortia publications for standard Legion use. 25/07/2012: now have a complete list from main users of Legion. To be discussed with CG when she returns from leave. 10/09/2012: CG to provide update on next meeting re linking and tagging enabling research content to be dynamically generated to allow readily refreshed content. CLOSED	NK
88	Consolidated metrics and information for reporting and users	(24/05/2012): Merge items 70,79,83,84,85 and report at next meeting 70 – (26/06/2012): ONGOING <ol style="list-style-type: none"> 1) Total node utilisation – The amount of time a node is being utilised by any job vs. total up-time (simple binary measure per node) summed over all nodes. 2) Used/requested memory – The ratio of effectively utilised memory to requested memory. 3) Requested memory vs. Requested cores plotted over time – Simultaneous (side by side) plot of CPU and memory utilisation over time, possibly normalised for each component. <p>Points 1 and 3 have now been implemented as database entries and the RC team is now working on presenting these as a report. Implementation of Point 2 requires further investigation.</p> <p>25/07/12 – Database entries are now ready and will be presented at next meeting.</p> <p>83 - (26/06/2012)</p> <p>To provide report and analysis on the Serial vs. Parallel parts of the system for top 5 users.</p>	BCS

		<p>25/07/2012 - DONE</p> <p>It was agreed that a discussion needs to be had at a later date, in the form of a presentation at a future meeting, about what information is made available to users and what information is made available to the group – add item to agenda.</p> <p>85 - (26/06/2012): ONGOING</p> <p>Develop simple utilities of transparency for infiniband jobs, a simple map of what is running and where.</p> <p>25/07/2012 – ONGOING</p> <p>(12/10/2012): Note that in future discussion in meetings re usage should be 'by exception', with all members to review reports using online tool (link has already been circulated) prior to each meeting. Next step will be to extract data from scheduler for live up to minute reporting.</p>	
90	Provide information to CRAG about backfill policy and job characteristics of top user.	<p>(25/07/2012) – Action requested</p> <p>Requested to clarify whether the job distribution observed in July was due to backfill settings and user job profile.</p> <p>(10/09/2012): BCS to provide data/stats for backfill jobs.</p>	BCS
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>	TC
92	Review of next version of KPIs' 'strawman'	Re-edit KPIs document and present to WG1 Research Computing working group.	CG
93	Automatic Extraction of Legion generated research papers.	<p>(12/10/2012): VP to experiment via automatic extraction to identify and search Legion generated research papers on web. Also suggested tagging e.g. Legion@UCL.</p> <p>(12/10/2012)CG to send webpage publications lists to consortium leaders.</p>	VP CG