

RESEARCH COMPUTING WORKING GROUP (RCWG)

MINUTES

Date: Tuesday 16th October 2012

Time: 12:00 – 14:00

Venue: Barlow Room, Roberts Building, Dept. of Electronic & Electrical Engineering,
UCL

Members Present:

1. John Brodholt [JBr] – Chair
2. Nick Achilleos [NA] – Astrophysics Miracle Consortium
3. Daniel Buchan [DB] – (representing: David Jones – Bioinformatics)
4. Richard Catlow - Dept. of Chemistry
5. Peter Coveney [PV] – Computational Life and Medical Sciences (CLMS)
6. Clare Gryce [CG] – ISD Research Computing
7. Thomas Jones [TJ] – ISD Research Computing
8. Nora H De Leeuw [NDL] – Thomas Young Centre
9. Nik Kaltsoyannis [NK] – Chair of the CRAG
10. Jacky Pallas [JP] – Platform Technologies
11. Ben Slater [BS] – Chemistry (representing: Angelos Michaelides – Thomas Young Centre)
12. Ian Sillitoe [IS] - (representing: Christine Orengo - Structural and Molecular Biology)
13. Bruno Silva [BCS] – ISD Research Computing

Apologies:

14. Mat Disney – Geography
15. David Jones – Bioinformatics
16. Angelos Michaelides – Thomas Young Centre
17. Christine Orengo – Structural and Molecular Biology

Outline Minutes, items decisions taken and Actions agreed are provided below.

Matters Discussed

1. Approval of Minutes of previous meeting (27th April 2012)

The draft Minutes of the previous meetings of the group held on 27th April 2012 were approved.

2. Update on status of Actions from previous meetings

The list of current actions from the previous meeting was reviewed and updated.

3. Review of RCWG Terms of Reference

3.1. The Group reviewed and agreed the proposed terms of reference document previously circulated by CG

(See RCWG_16Oct12_ToRs.pdf)

The group queried whether the use of the term 'Working Group' was really appropriate to the remit and purpose of the group. CG noted that the group had originally been convened as a 'working group' to provide input on a specific issue, but agreed that the group (and the other WGs reporting to the RIISF) were now more standing advisory groups. It was also noted that the new governance groups for Research Software Development were to be called the RSD 'Executive' (peer to the CRAG) and the RSD 'Board' (peer to the RCWG). CG suggested that this discrepancy would likely come up at the RIISG, where hopefully it would be resolved.

Other aspects of the proposed ToRs were approved.

4. Report from CRAG

4.1. NK reported that the membership of the CRAG were being reviewed to represent the main users of each Consortium and would seek appropriate representation. (See Action item 16).

New CRAG members are as follows:

- Dr Nicholas Achilleos - Astrophysics and Remote Sensing
- Dr Vincent Plagnol – Next Generation Sequencing
- Prof Dario Alfe - Thomas Young Centre (Materials Science)
- Prof Andrew Philips - Epidemiology

4.2. NK reported that 40 research papers had been received from the Consortium Leaders citing research work using Legion. (See Action item 12)

4.3. NK highlighted the importance of capturing output from users in order to set appropriate thresholds. NK informed everyone of the online CRAG reporting tool to generate usage reports for both the CRAG and eventually users in order that they may monitor their own usage. (See Action item 11 & Agenda item 8b)

5. Report from ISD on current Projects and key service development activities:

- **Legion IV Project Phase 1**
- **Condor Service development**
- **Online reporting and service status tools**

- 5.1. BS explained Legion IV Project Phase 1a, hardware had been tested, configuration problems had been detected and resolved and the system was ready for service testing. Phase 1b to upgrade compute nodes to new version of Lustre clients only was to be initiated at the end of the production testing period.
- 5.2. BS highlighted that the team would be working with users utilising R and Python on Legion and would explore workloads that could be moved onto Condor. BS explained that work was underway to improve the usability of the Condor service on the Myriad desktop service. A new build/submission node to sit within Legion was also to be created. The team would also investigate the possibility of integrating future desktop compute resources into to the Legion environment, with access via Legion scheduler, running virtual nodes and offering full binary compatibility.
- 5.3. BS clarified that CRAG reports were now presented online using a report tool specific to CRAG needs. Some reports would be made available to users however the CRAG is yet to decide which ones. Live service status information particular to each user would also become available via the Research Computing webpages.
6. **Centre for Innovation (Cfi)** (see document: Centre for Innovation and Review of Proposed UCL Access policy, file name: LegioRCWG_16Oct12_pdf)
 - **Status update**
 - **Review of proposed UCL access policy**
- 6.1. An analysis of HECToR data done by HPCx at Edinburgh showed that wait times increased considerably once utilization increased above 80%. As a result, EPSRC is considering setting a target for the maximum utilization of HECToR of 80% of the theoretical maximum. UCL may want to think along those lines too. JB would present detailed data at the next meeting. (See new action 22)
- 6.2. The group reviewed the proposed UCL access policy. CG explained the Cfi functions and the document rationale. If UCL required a large scale, shared level machine, then this would need to be demonstrated. NA enquired as to what evidence would be required to best demonstrate this requirement? For instance, would the number of applications submitted to the CRAG to use Cfi facilities be evidence enough to justify UCL purchasing large scale, shared level machine.
- 6.3. NDL enquired as to whether industrially supported work should be noted on the application form, as this would encourage industrial engagement for research funding. RC highlighted the benefits of bringing on board industrial linked users to use Cfi facilities. JP noted that there could be issues in making some commercial software packages available to industrial users, specifically if these software packages had been purchased under academic licenses.
- 6.4. It was agreed to make the following amendments to the application form:

(See action 23 below).

- **Under Administrative Information, Domain Section:**
Create link to list existing research computing consortia in the Domain section of the application form. JP also suggested that IRIS themes could be used here, CG agreed to look into this.
- **Under Computer Task Information:**
Why is Emerald, IRIDIS or both the most appropriate machine(s) to use?

7. Legion IV Phase 2 (compute expansion) – options and recommendation (See Document: Agenda 7- Legion Phase 2; Budget Options and Recommendations. File name: RCWG_16Oct12_LegionIVPhase2.pdf)

- 7.1. CG presented a paper which set out recommendations, explaining the proposals for budgetary allocation changes since the last meeting in April. It was noted that all bids were submitted via the competitive bids process which resulted in prioritised bids and numerous cuts. Legion IV budget was cut by £300k and the off-site HPC budget cut by £107k, hence the total compute budget for 2012/13 was £895k. Therefore, it was not possible to take forward off-site HPC Phase 3 and Legion IV development. It was suggested to move forward with a focus on expansion and extension of the on-site facilities, with the main objective to consolidate Legion located at the Torrington Place Data Centre. CG also suggested that as a budget had not been allocated for an Off-site HPC, it would be prudent to investigate full utilisation of the Cfl facilities and services. CG highlighted that off-site HPC would be re-visited in 2013/14.

RC suggested that a three year agreement be put in place at UCL to commit funds to the running costs of the Cfl, to ensure that in future years it would not be necessary to use funding allocated to other projects. CG explained that funding for this had already been identified and secured for 2013/14 and that the need to use budget from other projects had been a one-off.

- 7.2. All other aspects of the proposed paper were accepted.

8. AOB

- 8.1. JB raised the subject of the impact of strategic collaborations on research facilities. DJ suggested combining costs of using research facilities via an agreed contract with a caveat to reserve services to UCL based users only. Any exceptions would be dealt with on a case by case basis.
- 8.2. There was a brief discussion regarding use of Legion and other Research Computing Platform services by UCL Honorary staff. DJ suggested that application form be amended to specify whether users are honorary members of staff.

- 8.3. JP noted the need for coordination between the Research Computing and Research Data teams; CG explained that these two groups work closely together within ISD and that once the Research Data pilot service was in place there would be opportunity for the groups to collaborate further in future service design. It was suggested that Max Wilkinson (Head of Research Data services) be asked to give a presentation at the next meeting (See new action 24)

9. Next Meeting Date

- 9.1. The next meeting will be on 21st March 2013 from 12noon to 2pm, Venue to be confirmed

9.2. Agenda Items:

- Use of Legion by IoZ and other honorary staff. CG to provide data of UCL honorary staff using Legion, across UCL.
- Review of Legion application cycle and need for annual re-application process.
- Review funding and project portfolio.

List of Current Actions

Shaded Actions will be deleted after next meeting.

No	Date	Minute	Owner	Action	Status and Notes
5	18/11/11	1.6.1	LRAW (Legion Resource Allocation Group, precursor to RCWG)	Establish policy for cluster/consortia leaders.	OPEN 6/2 – no progress 27/4 – no progress. Need to consider which group should own this action (CRAG or RCWG) 16/10 – agreed that the CRAG should own this action
6	18/11/11	1.7.1	CG	Progress discussions within ISD regarding research computing use of Desktops.	OPEN 6/2 – this is in progress within ISD 27/4 – still in progress with ISD; ISD to report when significant progress has been made
10	06/02/12	4.1	NK	CRAG to discuss handling of 'large users; set appropriate threshold above which a report on usage will be required. Design report.	OPEN 27/4 – referred back to the CRAG for recommendation Ownership changed to NK as new Chair or CRAG 16/10 – agreed that this should be linked to the account application/re-application process
11	06/02/12	4.2	NK	CRAG to give further consideration to allowing users to monitor their own usage and raise actions as appropriate.	OPEN 27/4 – ownership changed to NK as new Chair or CRAG 16/10 – to be discussed at next CRAG meeting
12	06/02/12	4.3	NK	CRAG to give further consideration to how researchers can be encouraged to make proposals for ambitious use of Legion, how this might be managed, and report back.	OPEN 27/4 – ownership changed to NK as new Chair or CRAG
13	06/02/12	4.4	NK	To provide data regarding use of Legion by taught students.	OPEN 27/4 – ownership changed to NK as new Chair or CRAG. Need for policy regarding use of Legion by taught students agreed.

					16/10 – CRAG is awaiting data to be provided by ISD Research Computing
14	06/02/12	4.5	CG	To further develop Resource Allocation Framework proposal: detail steps for implementation, communication to CRAG, confirm whether sign-off by RIISG is required.	OPEN 27/4 – RIISG have agreed no further sign-off needed. ISD to report back on considerations for implementation (see Minutes 6.1 and 6.2 above) 16/10 – Close
15	27/04/12	2.1	CG	Legion account application form to be amended to indicate whether applicant is taught student or not.	27/4 – action opened 16/10 – devolved to CRAG
16	27/04/12	3.2	NK	Review membership of CRAG and report back	27/4 – action opened 16/10 – see Minute 4.1. Completed. Close
17	27/04/12	6.2	RCWG	To consider at future meeting; whether projects that do not have direct funding for compute resources but bring in large overhead income should be given access to dedicated or ‘priority’ resources.	27/4 – action opened 16/10 – to discuss at future meeting
18	27/04/12	6.3	CG	Consult Research Services to confirm what costs can actually be put on grants, also with regard to need to align allocation periods and processes with the research services costing.	27/4 – action opened 16/10 – CG to do by next meeting
19	27/04/12	7.3	CG	To seek clarification from RIISG regarding relationship of ISD bid process to Research Equipment Funding round.	27/4 – action opened 16/10 – no progress to report
20	27/04/12	7.5	CG	To seek clarification where infrastructural operating costs for the offsite HPC would be met from in long term.	27/4 – action opened 16/10 – no progress to report
21	16/10/12	3.1	JB	To seek approval from RIISG to change name from Working Group to Executive.	16/10 – action opened

22	16/10/12	6.1	JB	To provide utilisation, usage and throughput data for HECToR	16/10 – action opened
23	16/10/12	6.4	CG	Apply changes to Cfl Application Form, circulate both policy and application form to users by end of October.	16/10 - action opened
24	16/10/12		CG	CG to request Max Wilkinson to give presentation at next meeting.	16/10 - action opened