EPSRC UK National Service for Computational Chemistry Software at Imperial College London

Funding period: 1st February 2011 – 31st January 2016
EPSRC Reference: EP/J003921/1

Key Performance Indicators (KPI) for the period of 1st February 2014 to 31st January 2015

	Feb-Apr 2014	May-Jul 2014	Aug-Oct 2014	Nov 2014-Jan 2015
A) No. of Separate Uni. Res. Group	70	74	64	77
B) Percentage Uptime of Total Available Time	Columbus 99.6%	Columbus 99.6%	Columbus 90.6% Slater 99.9%	Slater 99.39%
C) Percentage of Training Requests Responded to within Stated Window	100%	100%	100%	100%
D) Percentage of Training Requests Delivered within Stated Window	100%	100%	100%	100%
E) Percentage of Computer Access Requests Responded to within Stated Window	100%	100%	100%	100%
F) Percentage of Computer Access Requests Accepted	100%	94.4%	94.4%	100%
G) Average / Peak Loading	Columbus 73.62% / 99.4%	Columbus 61.1% / 100%	Columbus 5.0% / 34% Slater 47.9% / 83.5%	Slater 44.6% / 97.38%
H) Number of Customer Complaints / Approvals*	0/0	0/0	0/0	0/0
I) Number of Publications**	3	11	12	49

*No complaints/approvals received from users. An annual user survey has been sent to users (See 4_NSCCS_User_Survey_2015.pdf for details.) **Publications reported during the period (See 2_Publications_Reported_Year4.pdf for a full list). ^^More processes eligible to run than available CPUs. If there are more threads than CPUs some threads will have to wait for a slice of

a CPU to be allotted before that can do anything and the load average will be greater than the number of CPUs.

The KPIs are:

A) The Number of Individual Researchers and University Research Groups ["Users"] that have been in contact with Imperial College regarding EPSRC UK NSCCS (e.g. for advice, guidance etc) and/or have made use of the EPSRC UK NSCCS Service in that Period. This should be expressed as a Total Number for that period (If it is possible to split the total number into EPSRC UK NSCCS Users and EPSRC UK NSCCS Enquiries then this would be advantageous). The number reported is that of "Users" which have made use of the EPSRC UK NSCCS Service in that Period.
(The number reported is the total number of separate university research groups using the NSCCS during the period. This number does not include people who attended NSCCS Workshops that were opened to any UK academic staff, students and non-UK and non-academics. See 3_Summary_of_Training_events_Year4.pdf for full details of all training events.)

B) The Uptime (or Downtime) of the EPSRC UK NSCCS Equipment within the period.

This will be expressed as a percentage of the Total Available Time within that Period.

C) Percentage of Training Requests Responded to within Stated Window

D) Percentage of Training Requests Delivered within Stated Window

E) Percentage of Computer Access Requests Responded to within Stated Window

F) Percentage of Computer Access Requests Accepted

G) Average / Peak Loading (See Figures 1-4 for details)

H) Number of Customer Complaints / Approvals (See 4_NSCCS_User_Survey_2015.pdf)

I) Number of Publications (including examples of Key Publications with acknowledgement of EPSRC UK NSCCS Service) (See 2_Publications_Reported_Year4.pdf)

J) Annual Data - Identification & Load of Software usage (See Figure 5 and Table 1 for details)

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation (See Figures 6-8 for details)

G) Average / Peak Loading

The ganglia load graph shown in Figure 1 and 3 give the load (CPUs in use) of the machines for the period of 1st February 2014 to 31st January 2015.

Figure 2 and 4 show the CPU time used via the queuing systems for the period of 1st February 2014 to 31st January 2015.

Columbus

The Altix UV1000 has 512 CPUs with 480 dedicated to batch work. This gives 80,640 hours a week. Working on an overall average for the year of 98% of time being scheduled availability, i.e. approx. 8 days a year outage for scheduled developments, etc., this gives 78,868 as the weekly available hours.

Columbus was withdrawn from service on 30th September 2014.

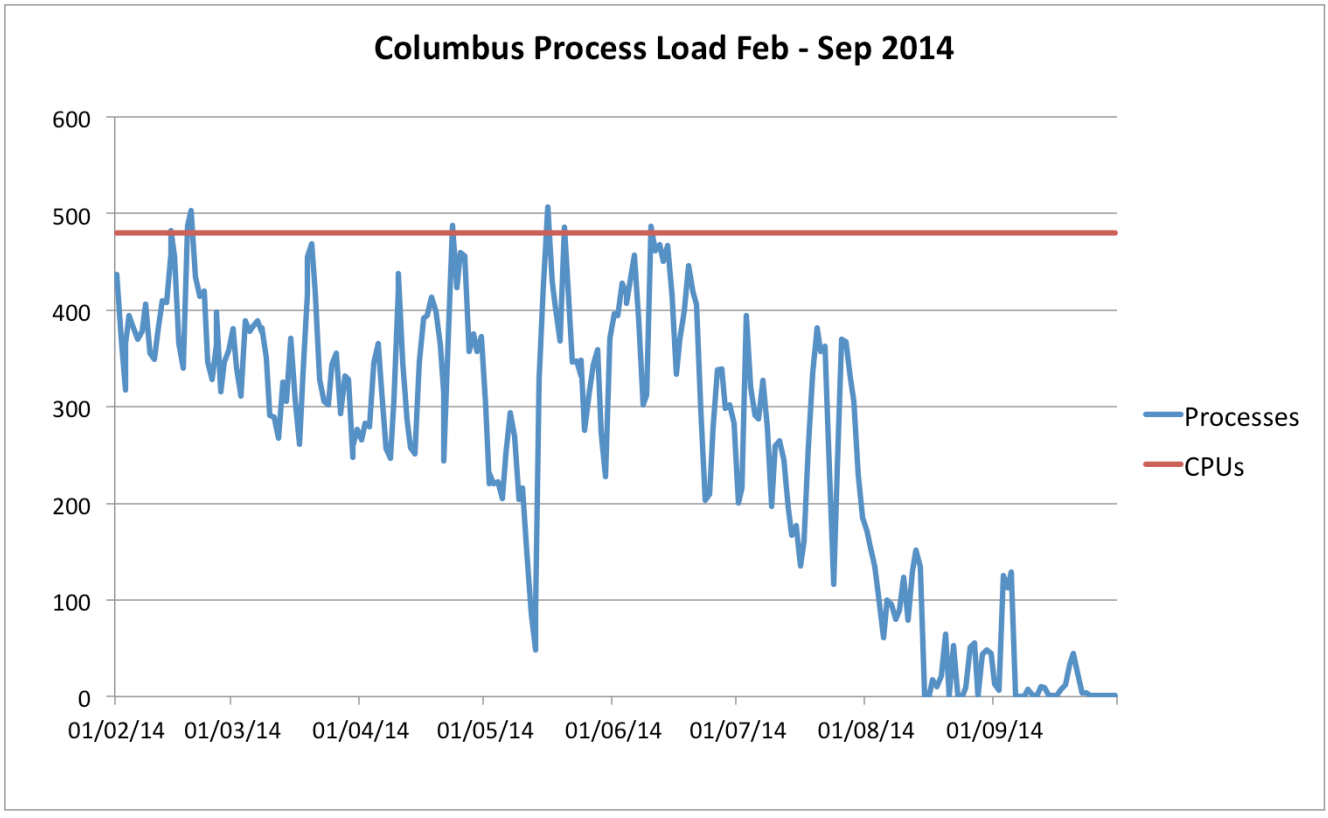

Figure 1. Ganglia load of NSCCS machine (Columbus).

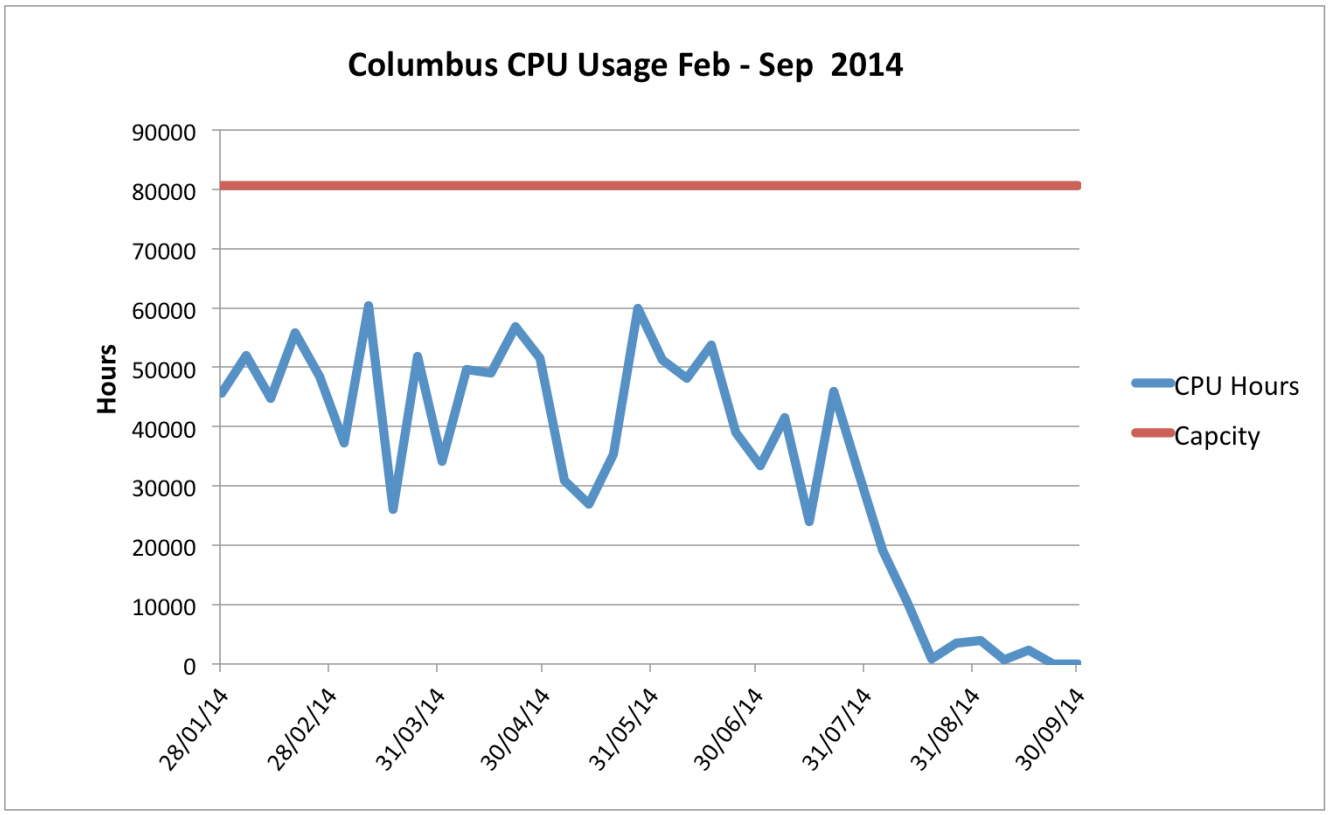

Figure 2. CPU usage of NSCCS machine (Columbus).

Slater

The Altix UV2000 has 512 CPUs with 480 dedicated to batch work. This gives 80,640 hours a week. Working on an overall average for the year of 98% of time being scheduled availability, i.e. approx. 8 days a year outage for scheduled developments, etc., this gives 78,868 as the weekly available hours.

Free trial of Slater started on 16th June 2014 and ended on 13th July 2014.

Charging against user CPU allocations started on 21st July 2014.

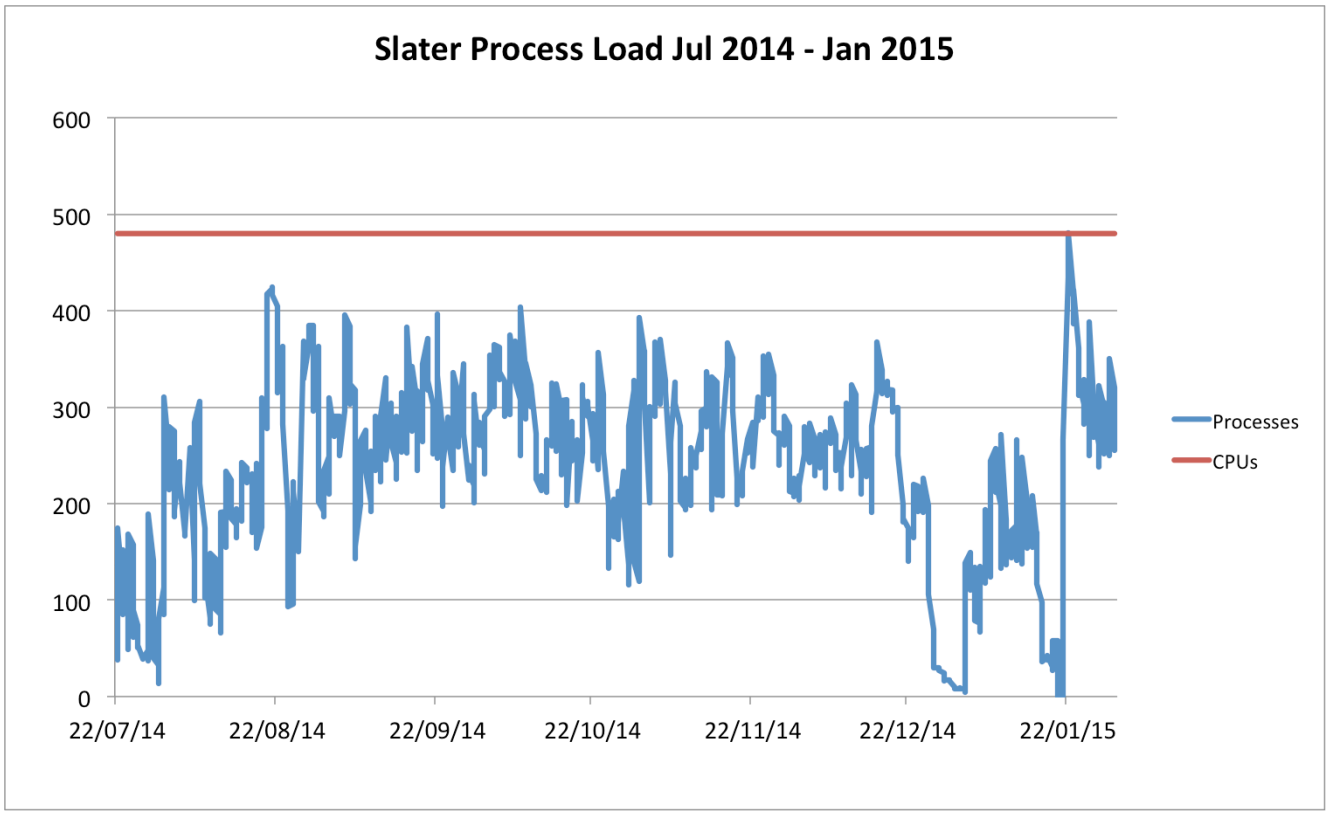

Figure 3. Ganglia load of NSCCS machine (Slater).

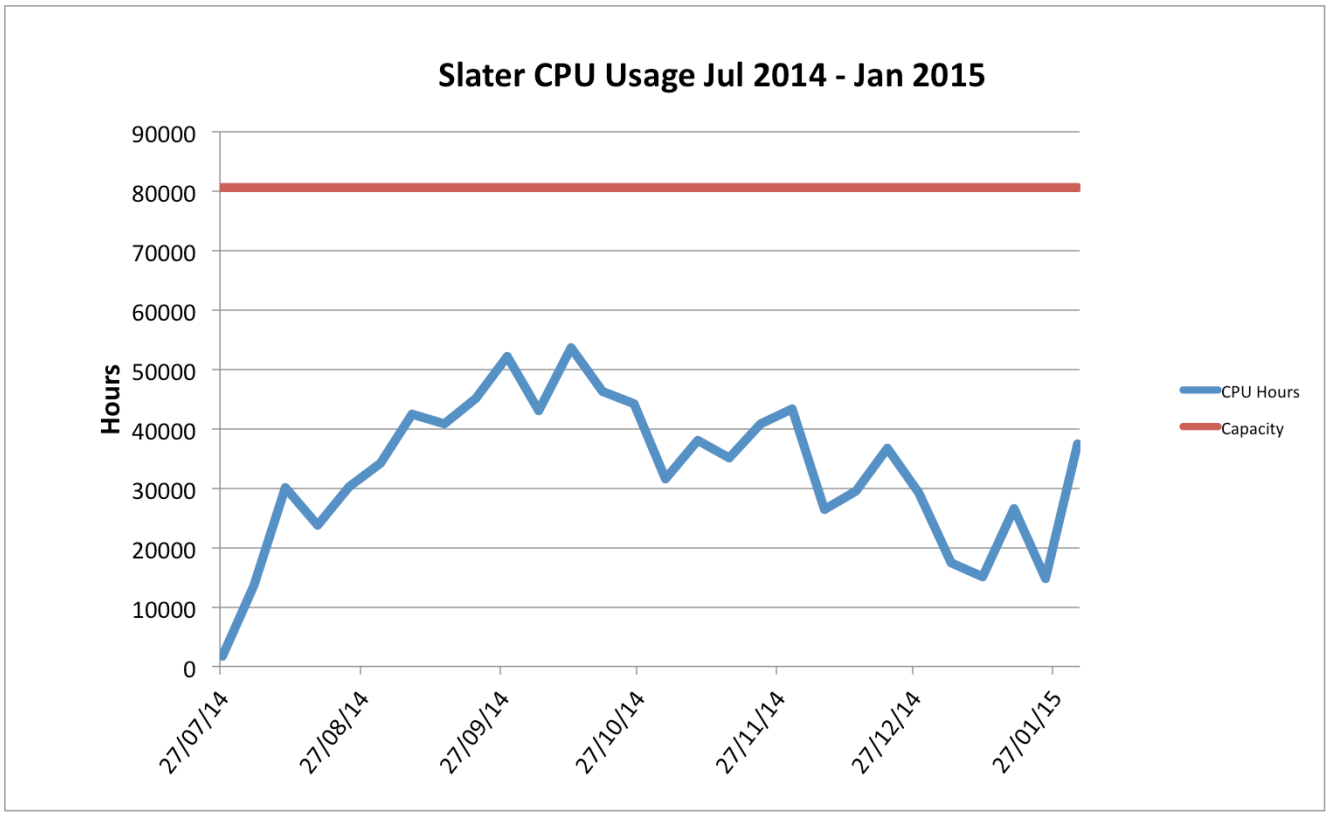

Figure 4. CPU usage of NSCCS machine (Slater).

J) Annual Data - Identification & Load of Software usage

The most used software package in terms of computing processing unit (CPU) is Gaussian at 65% as shown in Figure 5. The list of software packages' usage as a percentage is shown in Table 1.

*Please note that this is only for illustrative purpose since the logusage script used to gather the data cannot account for all parallel CPU usage. However, the actual CPU usage would have been accounted for by the system.

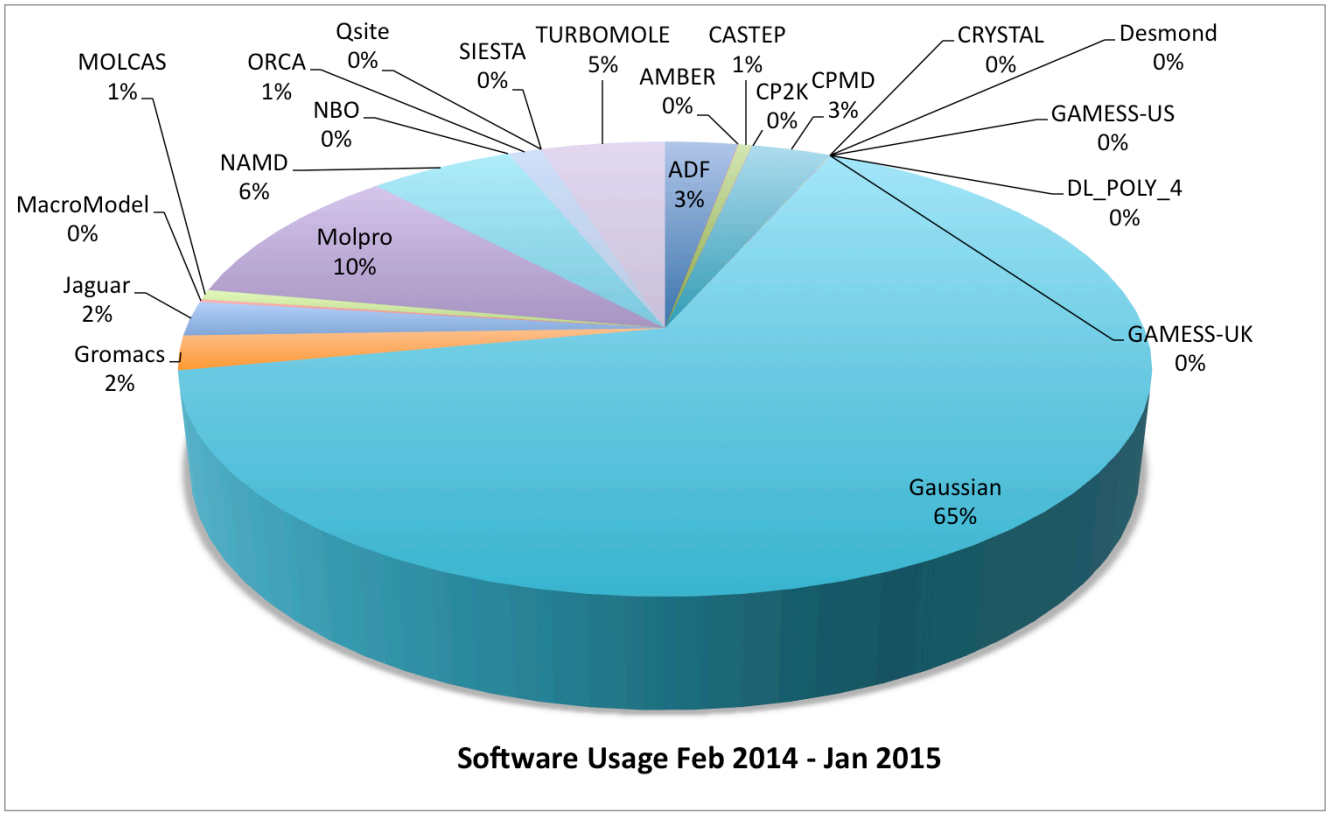

Figure 5. Software usage for the period of 1st Feb 2014 to 31st January 2015.

Software	Software Usage (%)
ADF	2.8697
AMBER	0.0294
CASTEP	0.5395
CP2K	0.0276
CPMD	3.1046
CRYSTAL	0.0001
Desmond	0.0072
DL_POLY_4	0.0001
GAMESS-UK	0.0160
GAMESS-US	0.0216
Gaussian	65.4123
Gromacs	2.4457
Jaguar	2.4650
MacroModel	0.2077
MOLCAS	0.7089
Molpro	10.2007
NAMD	5.7126
NBO	0.0002
ORCA	1.3164
Qsite	0.0005
SIESTA	0.0016
TURBOMOLE	4.9126

Table 1. List of software packages' usage for the period of 1st Feb 2014 to 31st January 2015.

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation

The NSCCS received 65 applications during the period of 1st February 2014 to 31st January 2015 with 22 pump-priming applications and 43 full applications; two were rejected, from 54 separate research groups from 24 institutions.

Figure 6 gives a breakdown of the number of research groups per institution from the 63 approved applications. The pie charts in Figures 7 and 8 illustrate the percentages of the different departments and different research categories of the research groups.

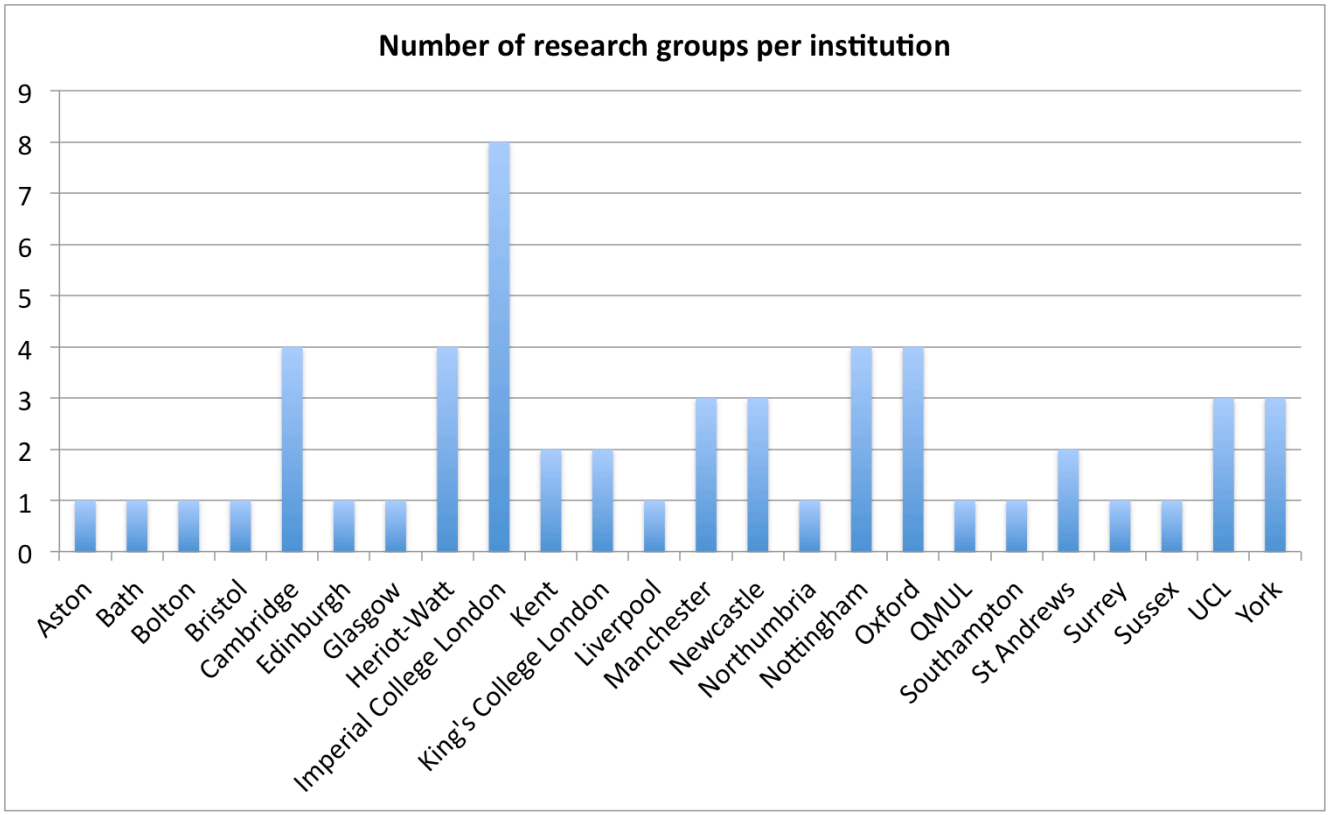

Figure 6. Number of research groups per institution.

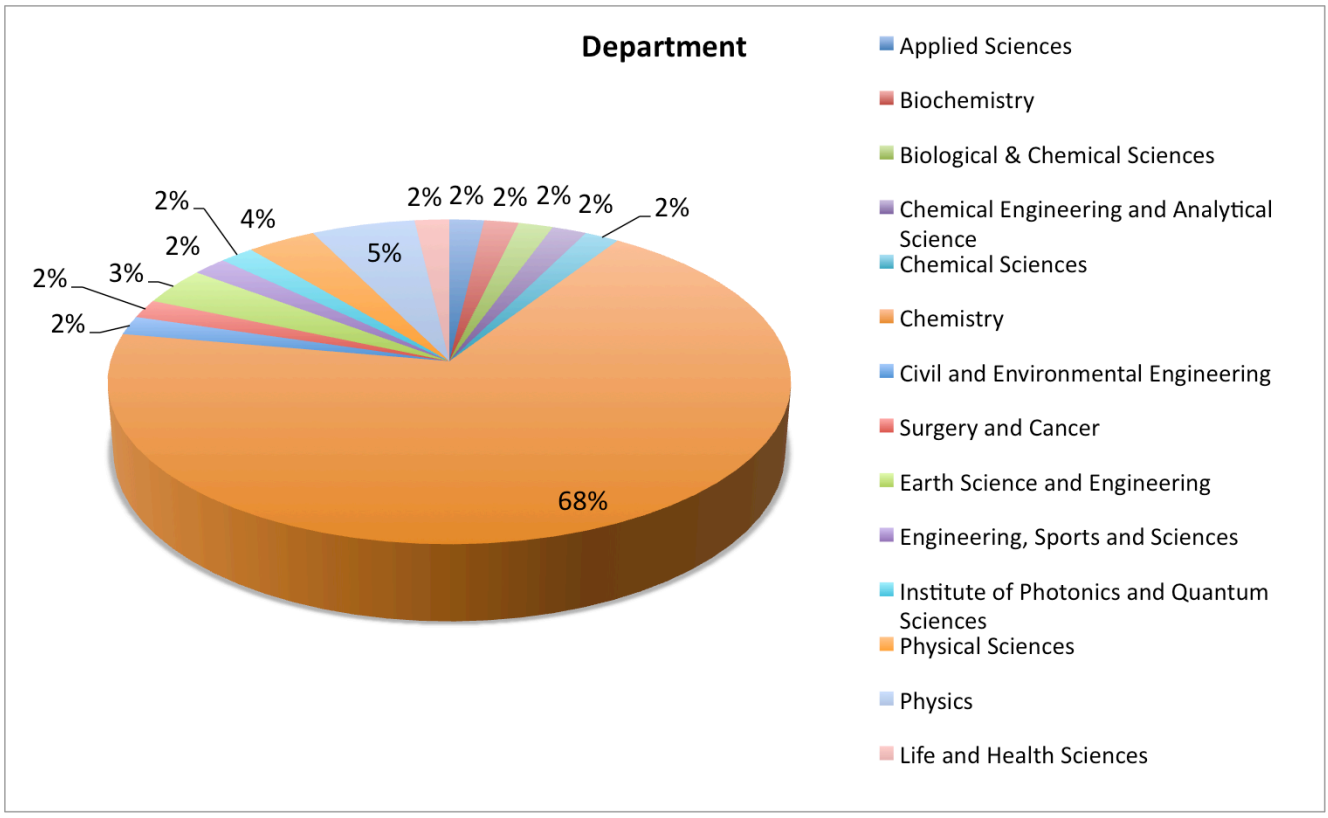

Figure 7. Users' department listed as a percentage.

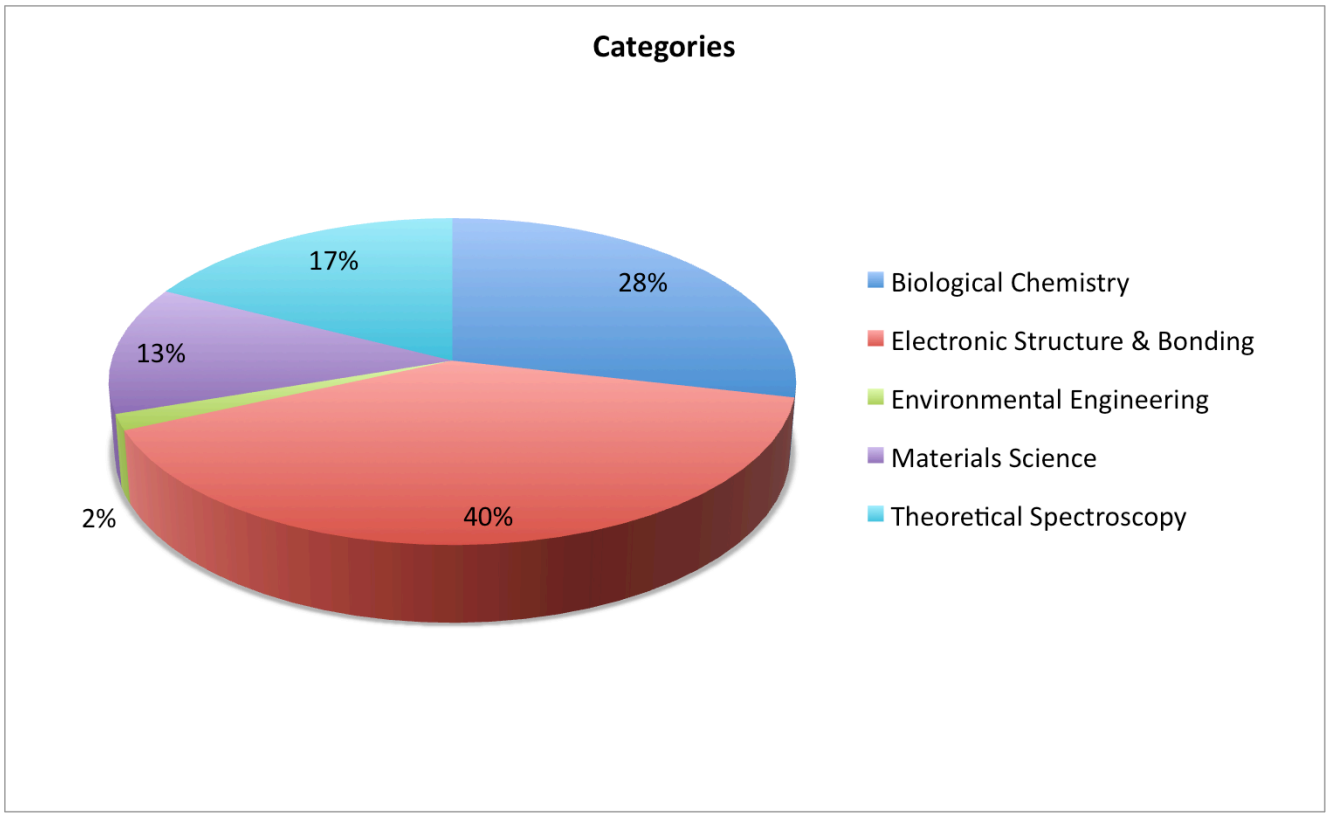

Figure 8. Research categories listed as a percentage.