

## 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

**Table 1. Key Performance Indices for the period of 1<sup>st</sup> February 2011 to 31<sup>st</sup> January 2012**

	<b>Feb-11 to Apr-11</b>	<b>May-11 to Jul-11</b>	<b>Aug-11 to Oct-11</b>	<b>Nov-11 to Jan-12</b>
A) No. of Separate Uni. Res. Group	18	20	29	44
B) Percentage Uptime of Total Available Time	100%	100%	100%	100%
C) Percentage of Training Requests Responded to within Stated Window	N/A <sup>^</sup>	N/A <sup>^</sup>	100%	100%
D) Percentage of Training Requests Delivered within Stated Window	N/A <sup>^</sup>	N/A <sup>^</sup>	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%	100%	100%	100%
G) Average / Peak Loading	Average of the 13 weeks was 17.5%, highest usage was 35% for week 17. The peak from the ganglia plot was around 87%.	Average of the 14 weeks was 19%, highest usage was 38% in week 27. The peak load from the ganglia plot was around 77%.	Average for the 14 weeks was 25%, highest usage was 52% in week 43. The peak load from the ganglia plot was around 78%.	Average for the 14 weeks was 54%, highest usage was 68% in week 47. The peak load from the ganglia plot was around 94% in early Nov and again in mid Jan.
H) Number of Customer Complaints / Approvals*	0/0	0/0	0/0	0/0
I) Number of Publications**	22	31	6	1

^The training programme started on 1<sup>st</sup> October 2011.

\*No complaints/approvals received from users.

\*\*Publication numbers were low in the 3<sup>rd</sup> and 4<sup>th</sup> quarters because most projects were set up in the current grant, we do not expect publications to be reported until these projects have been completed (From March 2012 onwards).

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).

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

H) Number of Customer Complaints / Approvals

I) Number of Publications (including examples of Key Publications with acknowledgement of EPSRC UK NSCCS Service)

J) Annual Data - Identification & Load of Software usage (See Figures 3 & 4 for details)

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation (See Figures 5, 6 & 7 for details)

### **G) Average / Peak Loading**

The ganglia load graph shown in Figure 1 gives the load of the machine for the period of 1<sup>st</sup> February 2011 to 31<sup>st</sup> January 2012.

Figure 2 shows the load of the queuing system for the period of 1<sup>st</sup> February 2011 to 31<sup>st</sup> January 2012.

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

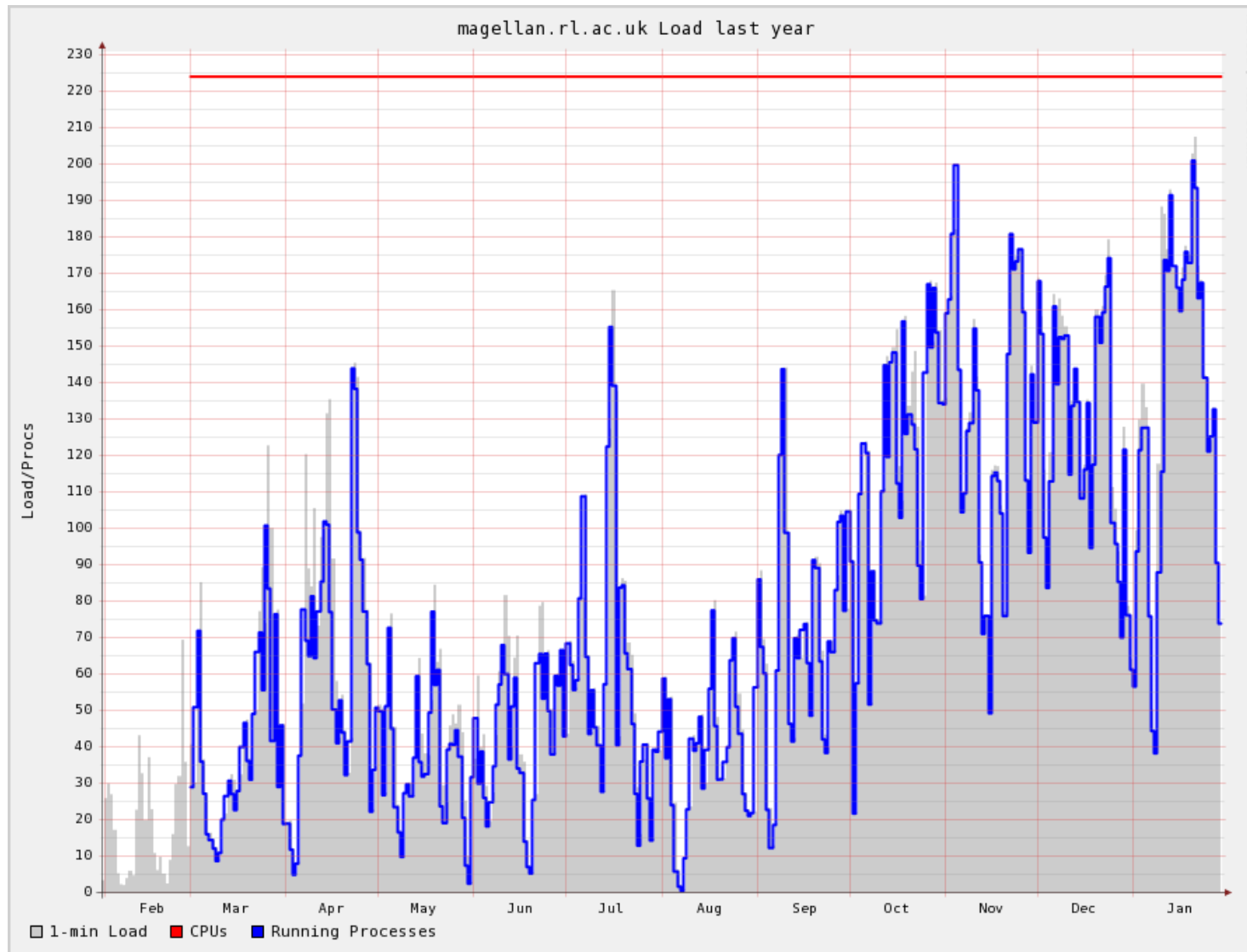
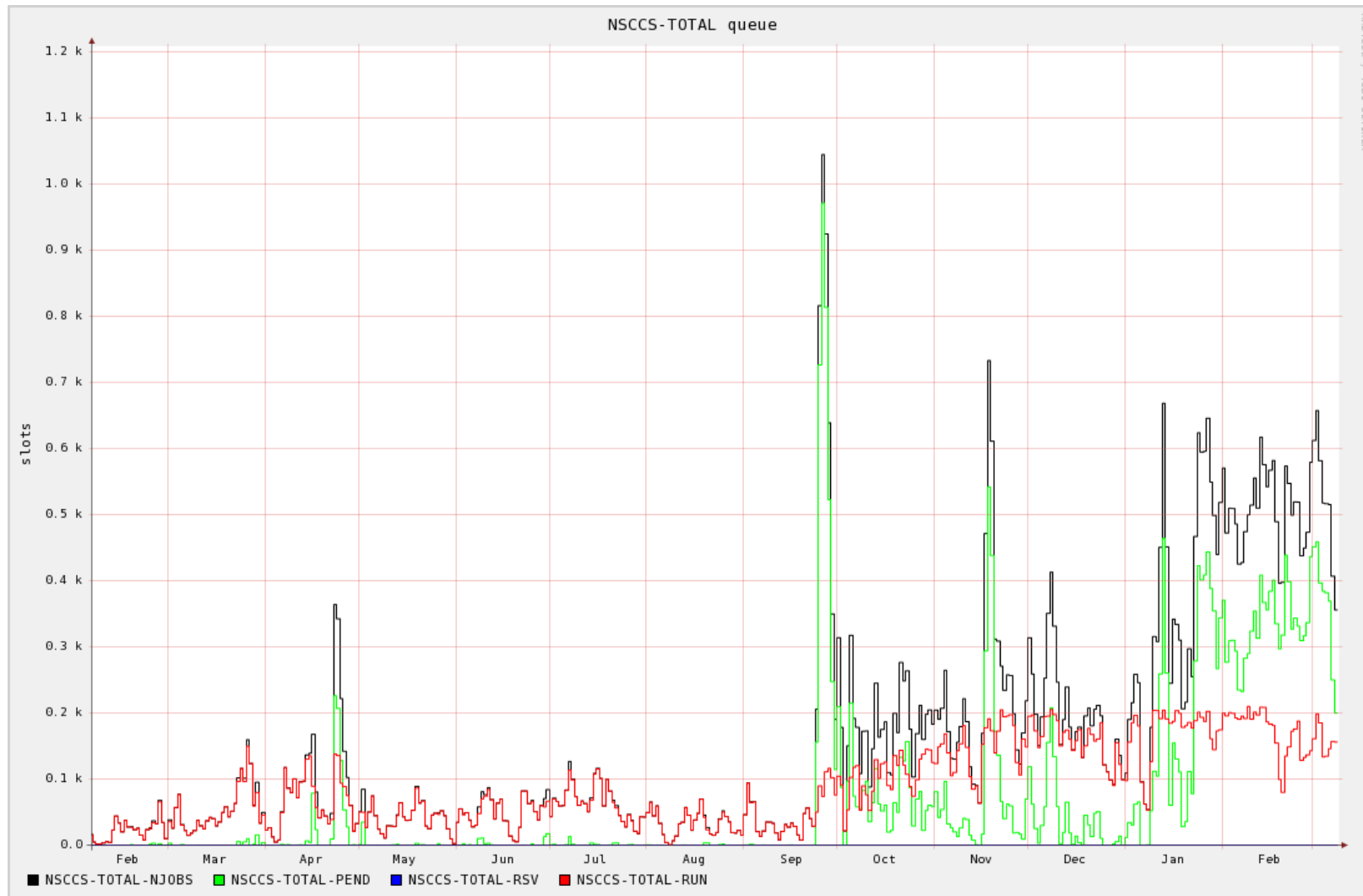


Figure 2. LSF batch load of NSCCS machine.

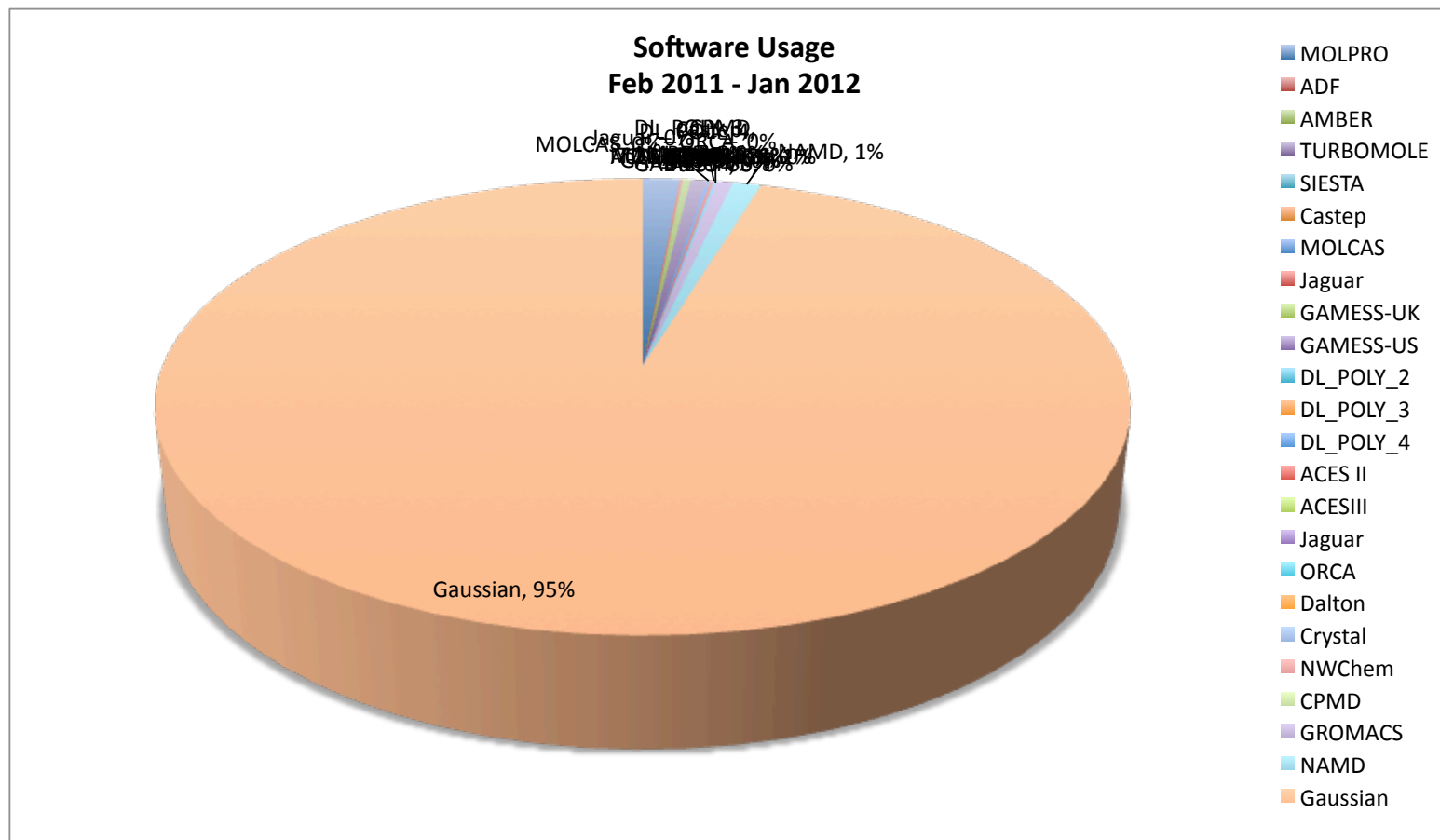


## J) Annual Data - Identification & Load of Software usage

The most used software package in terms of computing processing unit (CPU) is Gaussian at 95% as shown in Figure 3. The remaining 5% is shown in Figure 4 giving a break down of the other software usage.

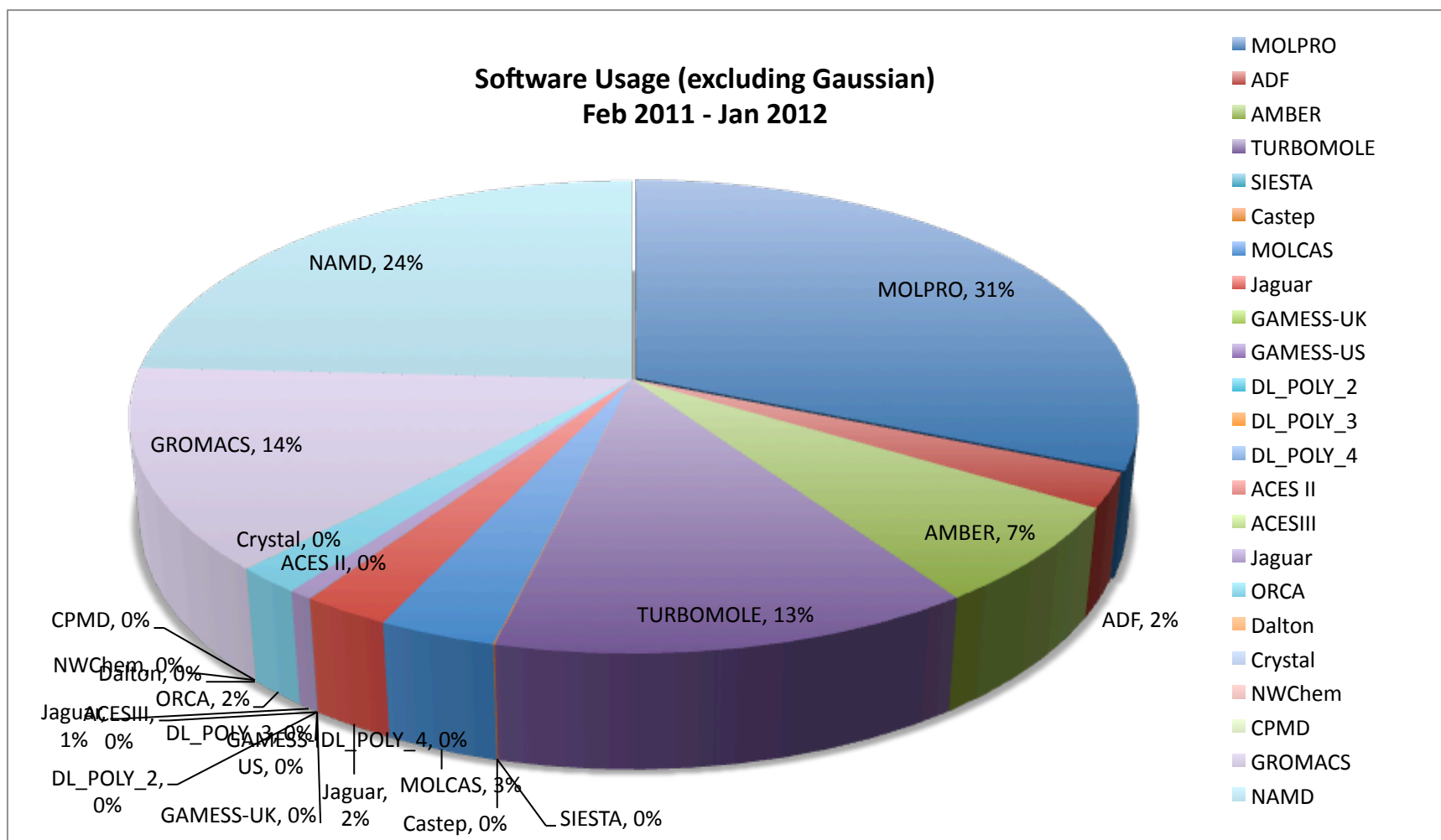
**Figure 3. Software usage for the period of 1<sup>st</sup> Feb 2011 to 31<sup>st</sup> January 2012.**

\*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 4. Software usage for the period of 1<sup>st</sup> Feb 2011 to 31<sup>st</sup> January 2012 excluding Gaussian.**

\*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.



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

The NSCCS has received 52 applications during the first year – 21 pump-priming applications and 31 full applications, from 45 separate research groups from 26 institutions. Figure 5 gives a break down of research groups per institution. The pie charts in Figures 6 & 7 illustrate the percentages of the different departments and different research categories of the research groups.

Figure 5. Number of research groups per institution.

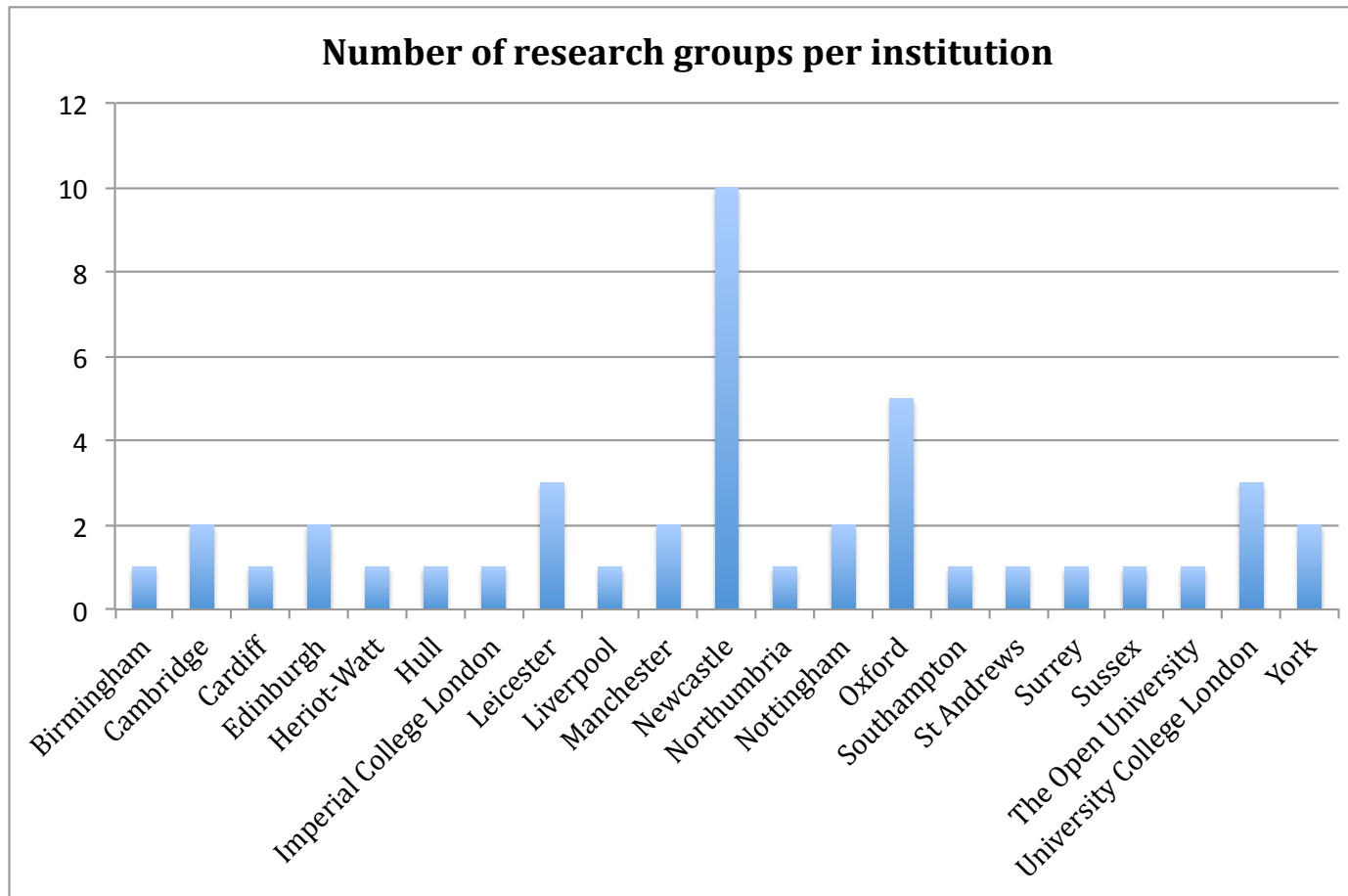




Figure 6. Users' Department listed as a percentage.

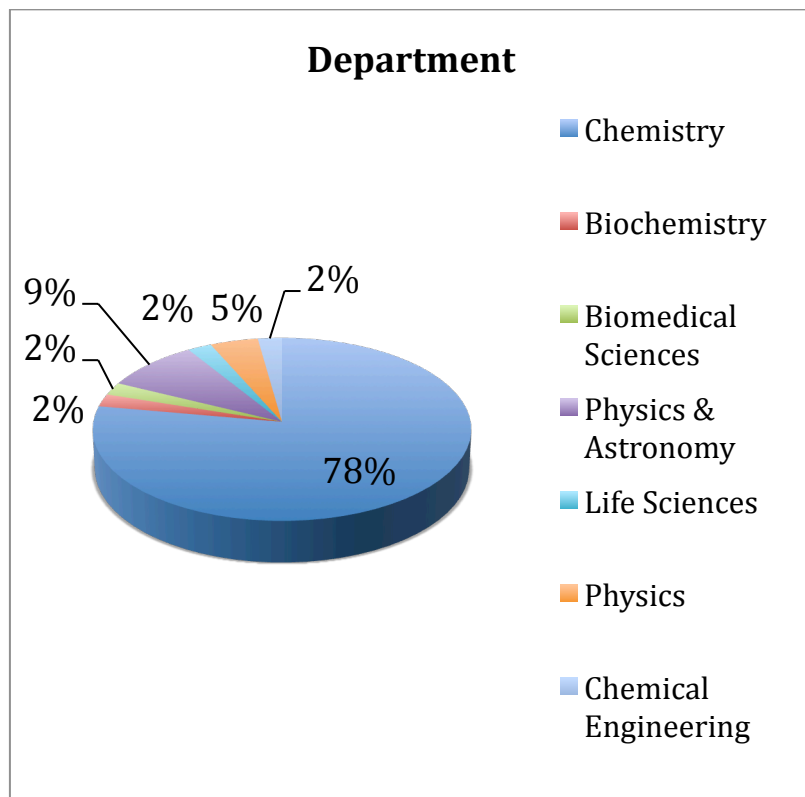


Figure 7. Research categories listed as a percentage.

