

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

NSCCS Annual User Satisfaction Survey 2016

In February 2016, the NSCCS asked all active users to complete the annual user satisfaction survey to evaluate the quality of the service provided for the period of 1st February 2015 to 31st January 2016. Questions asked in the survey are attached to the end of this document.

39 user surveys returned.

100% of users are satisfied with the overall support provided by NSCCS.

92.3% of users have rated the overall assessment of the Service as *Very Good* with 7.7% as *Good* (selected from *Very Good, Good, Satisfactory, Sufficient* and *Poor*).

Below list the optional "Other comments/feedback on the Service".

- I hope this service remains active in the future, it so useful to have access to this software where my institution/group simply does not - typically because of cost in the case of Turbomole and Gaussian09. This is allowing me to explore different complementary research areas to my experimental work.
- Alexandra Simperler is super helpful and approachable.
- I realise that the NSCCS is not really a hardware service, but I find calculations can run very slowly if they use lots of input/output. This is to the point where I would sometimes think about trying to buy software myself, rather than use the service.
- Very useful service for the computational (as well as experimental) community. Very approachable staff, very user friendly. Highly useful.
- Performance of CPMD is much quicker and more stable on Slater than it was on Columbus.
- Fantastic service.
- Many thanks.
- I am always very impressed by the friendliness, high level of professionalism and collaborative environment. It is a real pleasure.
- A valuable service which needs to be maintained at LEAST at the current level.
- This is an essential Service without which my research would be greatly hampered.
- The Service is essential to our research, which aims at pushing theory to its limit, and to complement and/or challenge experiments. Without the Service, we would not have collaborated with world renown experimental groups in USA and published a paper in Science.
- This really is an excellent service and underpins my group's ability to produce high-quality experimental publications supported by theoretical results.

- The one-on-one service provided by the NSCCS staff is exceptional. No question is too trivial, and they always take the time to explain how and why, rather than just provide you with a quick fix. I have found interacting with the NSCCS staff extremely beneficial to the progress of my research and look forward to working with them in the future.
- This service has proved invaluable over the years in allowing my group to access software and resources that would otherwise be unavailable to them.
- I hadn't used the service for 10 years or more until November 2015, and have only used it for small calculations since then, but I have found it much easier to use than I remember from before. It's very helpful to have program packages available which I don't expect to use very much but for which I would otherwise have to find a substantial payment.
- Exceptional levels of training were provided. The service is extremely encouraging for researchers who have little experience of computational chemistry but who would like to use it to enhance their research.
- Exceptionally good service!
- Extremely useful - especially for us as experimentalists and the support and guidance is excellent.
- It remains the envy of colleagues in other countries.
- The Service seems to be useful mostly for certain kind of jobs. Very large MD seems to take lots of time to enter the queue (according to my students).
- Great service, absolutely necessary especially for academics in universities with limited resources. Would be better if possible the MD codes (Gromacs, Amber) to be possible to run on more cores e.g. 128-256. it would be great to upgrade the service with more nodes and also GPU nodes for MDs. Advanced training on QM/MM using Chemshell would be great. Overall I appreciate very highly the opportunity to have access to the NSCCS and it is vital for my research. The staff is friendly and very supportive.

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It is important for the NSCCS to receive feedback from our users to evaluate on the service we provide. If you have been an active user between 1st February 2015 and 31st January 2016, we would be grateful if you could complete this annual user satisfaction survey to provide us with feedback and comments on how we performed in the past year.

Your feedback and comments will ensure the quality of our service to be maintained at a high standard and to help us make further improvements.

Please complete and submit the survey by Wednesday 24th February 2016. Please ensure all fields have been filled in unless indicated as optional. Many thanks for your help.

Annual User Satisfaction Survey

Title: (Mr, Ms, Professor, Dr, Others)

Name: (First Name, Surname)

Department/Group:

Institution:

Email:

1. Please list all the software packages that you have used and/or are currently using on the Service machines. Please indicate the main software package that you use.

2. Please list any software packages that you would have liked to have used, but are not available from the Service. (optional)

3. Did you request training for the software of your choice?

 Yes No

4. Have you attended any of our training workshops?

 Yes No

5. Would you be interested in attending future workshops?

 Yes No

If yes, which training workshop(s) would you be interested in attending?

6. Please indicate whether you were given sufficient information in the following areas:

Accessing the machine for the first time:

 Yes

No

Running jobs in the batch queues:

Yes

No

Running the software package(s):

Yes

No

If you answered "No" to any of the above, how did you solve your problem(s)?

by contacting the NSCCS staff and/or NSCCS Support Helpdesk (email: nsccs.support@stfc.ac.uk)

by looking on the NSCCS website/user guide

by asking another user

never solved the problem

other (please specify)

7. Have you ever visited our Service web site (<http://www.nsccs.ac.uk>)?

Yes

No

If yes, what was the reason for your visit(s)? (You may tick more than one box).

to download an application form

to look for information on using the machine

to look for information on using software

to look for information on using training/workshops

to look at the NSCCS user guide

just browsing

other (please specify)

8. Have you been satisfied with the overall support provided by NSCCS ?

Yes

No

9. Please give your overall assessment of the Service.

Very Good

Good

Satisfactory

Sufficient

Poor

10. Other comments/feedbacks on the Service: (optional)

