

Application Guidelines for EPSRC UK NSCCS Computing Resources

To apply for our resources, please complete the application form, append a description of your proposed research, and save it as a Microsoft Word document or Adobe PDF and return both by email to Dr Helen Tsui (helen.tsui@imperial.ac.uk). If you have any other questions regarding the application procedure, please send an email to the above address. Please note that your application cannot be processed unless all compulsory fields are filled. Below are some guidelines to help you complete your application.

Your application will be peer reviewed. If the review is successful, user registration details will be emailed to you, unless you already have a valid NSCCS userid. You will be sent a web link to sign electronically a Declaration Form agreeing to the NSCCS Terms and Conditions, STFC's data protection act and Security Instructions for Users. The 'NSCCS Terms and Conditions' can be found on our website at <http://www.nscs.ac.uk/termsfuse.php>

Eligibility

Any researcher eligible to apply for an EPSRC grant can apply for resources (see excerpt from EPSRC Funding Guide - August 2011 version below).

**Please note that postgraduate students and research assistants are not eligible to apply in person. If they wish to apply for resources, they must do so via their supervisor.*

Eligibility of Investigators

"Principal Investigators must be academic employees (lecturer or equivalent) of an eligible organisation and must be resident in the UK. EPSRC Fellows (except Postdoctoral Fellows) and Royal Society Fellows are also eligible to be Principal Investigators.

Principal Investigators should normally hold a permanent post but fixed-term employees may be eligible provided that the EPSRC can be satisfied that the host research organisation is prepared to give the individual all the support normal for a permanent employee and that there is no conflict of interest between the investigators obligations to the EPSRC and to any other organisation or employer. The term of employment of a fixed-term employee must extend beyond the duration of the proposed research project."

Please make sure you give a valid email address, as this will be our primary means of contact with you regarding your application.

Pump-priming accounts

Our service offers new users access to a small amount of resources (normally 100 CPU hours for 3 months duration) to try out the software packages, for use in training and also to estimate the amount of resources required for their project before submitting a full application. For pump-priming application, please complete the standard application form with your contact details, the title of your project and the software packages you wish to access. There is no need to submit a full project proposal at this stage.

Project details

You are required to submit a brief description of your proposed research (approximately 1-4 sides of A4 depending on the amount of CPU time requested). This should include:

- A summary of the scientific background to the research.
- A comprehensive breakdown of how you propose to use the CPU time requested. In your plan you should state clearly the calculations you wish to carry out (i.e. the systems of interest), the computational methods and basis sets (if applicable) that are to be used, and the relevant software packages involved.
- Details of any similar calculations you may have carried out previously on which you are basing your time estimate.

Project resources

Please note that the CPU time requested must be justified. Although we allow requests of up to 100,000 CPU hours per annum, applicants are asked to consider carefully the actual amount of time required for their project. This estimate should be based on previous experience where possible.

Please give details of CPU hours required for a typical job if known, including size of calculation and methodology used.

The default amount of disk space is currently set at 10 GB. This is normally more than adequate for most purposes. If you require more than this, please specify the amount.

Software requirements

Please list all the software packages you are proposing to use, as specified in your project details. Applicants are advised not to give a long list of software packages if they have no details of how these packages will be used.

Training requirements

We offer free one-to-one training sessions on most of our software packages. If you or members of your group/collaborators require training, please indicate which packages they would like training on and we will set up a training session as soon as possible.

Other grants

Please list any other grants you have associated with this project.

Reports

After you have used up your allocated resources, you will be asked to submit a short report to describe how you have used the time allocated to you and the results you have obtained. We will send you further details on what needs to be included in the report nearer the time. We also request that you acknowledge the use of the NSCCS in any presentations and publications that arise from your project. The official citation can be found at <http://www.nscs.ac.uk/citation.php>. We are required to submit the reports and publications to EPSRC to demonstrate the good work that has been carried out by users in the computational chemistry community. Please indicate that you agree to this by signing in the space given.

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