# Guide For DMU users of Cambridge HPC system.

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## Who should read this?

This is a guide for De Montfort University Faculty of Technology staff and research students using the High Performance Computing Facility at Cambridge. We have a contract with them for some limited use of their systems.

The Faculty of Technology provides a small budget to fund access to High Performance Computing (HPC) facilities for faculty staff and research students only, who are conducting research which is not externally funded. Computing resources for externally funded research should be procured separately

## General Description

This guide will largely be a collection of links to other resources. It is intended to collect enough information to reduce the "bus factor" of the project so that others can setup machines to join the project.

It will also function as a growing collection of knowledge. If you find out things that will be generally helpful to other people, let us know and we'll see if we can add the information or pointers to an authoritative resource.

## Getting an Account.

If you contact [Dr. Hugh Sasse](mailto:hgs@dmu.ac.uk) he can arrange for you to get an account. The form can be downloaded, but he will have most of the information you will need for it. Requests for a resource allocation for research students should come from the studentâ€™s supervisors. Please be aware that any software applications required, and access to corresponding licenses if appropriate, must be provided by DMU. You will need to supply:

* Your Name
* Your email address
* The IP address of your computer
* How many core hours you are likely to need
* Over what period you will be using the system

You will need to read some of the [Cambridge documentation](#cam_docs) below before you do this, in order to understand their policies, which are not unreasonable. In particular, the anti-virus systems on your machine must be up-to-date.

You will need to contact [ITMS](mailto:itmsservicedesk@dmu.ac.uk) on 6050 to arrange to have [Cygwin](#cygwin), [Cygwin/X](#cygwin_x) and [ParaView](file:///C:\hgs_documents\HPC_Cambridge\DMU_HPC_Cambridge_Guide\ParaView) on your PC.

When the form is complete, it is you who sends it off to the specified support address, because they contact you about your account.

The [Jira](https://en.wikipedia.org/wiki/Jira_%28software%29) help system from which you will receive notifications is not accessible outside Cambridge; attempting to access it will yield a connection error which looks rather like a certificate problem. You will encounter this at the first stage of setting up your account, before you are notified of the account name. You will also not receive the password by email. You are best obtaining that by telephone.

**Note:** There have been Phishing attempts aimed at Cambridge HPC users recently (APR-2017). Please be aware of this. These have used names of Cambridge staff to look convincing. If you have any problems of that sort, don't follow the links, but contact Cambridge support to let them know, unless they already do.

## Cambridge HPC Related Documentation

[Cambridge HPC Application Form For Institutions (i.e., us)](http://www.hpc.cam.ac.uk/services/applying-for-resources/hpc-application-industrial-doc).

This is a Microsoft Word Document download.

[Access to the Cambridge Network](http://help.uis.cam.ac.uk/devices-networks-printing/network-services/infoinstitutions/remote-introduction).

[HPC Privacy Policy](http://www.hpc.cam.ac.uk/policies/privacy-policy).

[Quick Start](http://www.hpc.cam.ac.uk/using-clusters/quick-start).

slurm uses [MPI](https://www.open-mpi.org/), (rather than the older [PVM](https://en.wikipedia.org/wiki/Parallel_Virtual_Machine)). The system uses Intel compilers. Use the module system to see what is available and to load more things if needed.

[Cambridge HPC FAQ](http://www.hpc.cam.ac.uk/getting-help/faq).

For the number of nodes question, which will keep coimg up, see "[What values should I choose for --nodes, --ntasks etc?](http://www.hpc.cam.ac.uk/getting-help/faq#section-9)".

## Cygwin Setup information

Cygwin is a Unix emulation layer for Windows. It provides a shell, and a collection of tools which can be downloaded (it does not provide all of them at the outset, because there are many). It is of interest to HPC users because it allows access to X Windows. Information on Cygwin can be had from [cygwin.com](https://cygwin.com/). The [installer/updater](https://cygwin.com/install.html) which is GUI based can be obtained from the same site, see the menu on the left.

## Cygwin/X Setup information

The X windows facility provided by [Cygwin](#cygwin) is obtained through the Setup program. Details of setting this up can be found in the [Cygwin/X User's Guide](https://x.cygwin.com/docs/ug/cygwin-x-ug.html) and in the [Cygwin/X Frequently Asked Questions](http://x.cygwin.com/docs/faq/cygwin-x-faq.html) document.

It is important to set the DISPLAY environment variable to something appropriate. A value of :0.0 seems to work, so something like:  
export DISPLAY=:0.0 in your .bashrc file in your Cygwin home directory should do the trick. It does for me, anyway.

Starting the server was one part I had wrong. I think it has changed since I last did much of this. The details are at [Starting in multiwindow mode (startxwin)](https://x.cygwin.com/docs/ug/using.html#using-starting-exe) but amount to using startxwin from the command line, or using the "XWin Server" shortcut under "Cygwin-X" . This may be better.

However, according to [Connecting to Darwin via TurboVNC](http://www.hpc.cam.ac.uk/using-clusters/remote-desktops-and-3d/darwin-turbovnc) which I received on account creation, we should be using a Virtual Private Network Connection.

## OpenFOAM information.

There seem to be two sources of OpenFOAM information, [openfoam.com](https://openfoam.com/) and [openfoam.org](https://openfoam.org/). You may need information from either site.

The [Installation and build Instructions](https://openfoam.org/download/source/) are available, but you should not need to put these on your machine, this is just for information, as is this mention of the [the git repository](https://github.com/OpenFOAM/OpenFOAM-4.x).

Bear in mind the [FAQ about using nice -n 19 on login nodes](http://www.hpc.cam.ac.uk/getting-help/faq#section-8) when building anything on those machines.

By using the command [module whatis](http://www.hpc.cam.ac.uk/using-clusters/quick-start#section-3) you can see we have these on the Cambridge system:

openfoam/4.1 : adds OpenFOAM 4.1 and Paraview 5.0

(GCC/Open MPI build) to your environment

([ParaView](http://www.paraview.org/) is a 3D graphics viewing package for data visualization.) So add:  
**module load openfoam/4.1**  
to the end of your .bashrc file. (You will also need this module mentioned in your submit file.)

This added some things to your path.  
OpenFOAM is a toolkit, it contains multiple executables(solvers, utilities) but not an executable called OpenFOAM. The best way to understand how it works is to look at some of the tutorials inside the OpenFOAM directory in conjunction with the online documentation from CFD Direct at: <https://cfd.direct/openfoam/user-guide/> The tutorials are inside $FOAM\_TUTORIALS and you can copy them to your home directory. The structure of the tutorials directory is:

tutorials/domain/solvers/case

Each tutorial case typically contains the following:

Allrun

script for executing the different steps of a simulation, parallel parts are run on a single node

Allclean

removes files which were created when Allrun was executed

0.orig

contains the configurations/initial conditions for variables which will be used. This will usually be renamed to "0" which stands for time 0 of the simulation.

system

contains the dictionaries for a case describing how it will be run such as runtime, IO controls, solver properties, decomposition, meshing.

constant

contains the different meshes, if it doesn't exist usually Allrun creates it by copying a mesh from the tutorials' resources directory.

There is a need to specify modules in the script which lauches batch jobs on the host called darwin.

When a job is launched SLURM will execute the job script on the first node of the list of nodes allocated, but will propagate many of the environment variables set during submission time. Also, because the bash shell at that time is neither a login shell nor an interactive shell, neither .bashrc nor .bash\_profile will be sourced. Because this means that the effective environment at job run time is not determined by the contents of the job submission script, and is determined only incidentally via the .bashrc through the environment at submission time which could include additional changes, we would recommend always specifying the desired environment explicitly in the job script to prevent surprise behaviour. (Even if the ~/.bashrc were a reliable method of controlling the runtime environment of batch jobs, it would be a clumsy global setting and a change to it could affect the behaviour of jobs submitted earlier, so this is still an inadvisable approach.) The template submission scripts under /usr/local/Cluster-Docs/SLURM contain the following logic:

. /etc/profile.d/modules.sh # Leave this line (enables the module command)

module purge # Removes all modules still loaded

module load default-impi # REQUIRED - loads the basic environment

#! Insert additional module load commands after this line if needed:

This resets the environment to the default and allows the user to specify changes relative to that known starting point.

In the scripts supplied, the mpirun command is invoked with a -ppn flag, which is not mentioned in the manual page man mpirun. This is an option of the mpirun wrapper script associated with Intel MPI, and Intel have not included a man page for it. The documentation can be found around the web but there is a reference guide in pdf form at  
/usr/local/Cluster-Apps/intel/impi/4.1.3.045/doc/Reference\_Manual.pdf

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