

Temporary Class Account

We have made an account for you on the machines at the Alabama Supercomputer Center. These systems are an SGI Ultraviolet, and a locally architected fat node cluster called a Dense Memory Cluster (DMC). Below is some information for new users of these machines. You can login, following the directions below, using the login and password provided by your instructor.

WARNING: This is a temporary account. The account and all the files in it will be deleted at the end of the semester.

The best source of information on using these computers is the HPC User Manual, which can be accessed on the web at

<https://www.asc.edu/files/HPC-User-Manual>

The command "ascdocs" shows a menu drive listing of locally written documentation. It displays text files, and gives paths for you to copy or download other types of files.

The computers can be accessed using secure shell (an encrypted form of telnet). Secure shell is installed on many Linux and Unix machines, and can be called with a command like this

```
ssh UserID@uv.asc.edu  
ssh UserID@dmc.asc.edu
```

The first time you login, you will have to enter the password a second time, then set a new password. You will also be asked to enter an email address where error messages can be sent. This should be a complete email in the form myname@myschool.edu

Files can be copied to and from the DMC using secure copy "scp" or secure ftp "sftp". These programs are often included with secure shell software.

You can get help from the Alabama Supercomputer Center staff at hpc@asc.edu or [\(256\) 971-7448](tel:256-971-7448) or [\(800\) 338-8320](tel:800-338-8320). The staff can help with using the applications on the computers, accessing the system, etc.

In order to get the maximum possible utilization of the computers, computational jobs are executed through the SLURM job queueing system. SLURM can be accessed via commands like "squeue" to check queue status.

Scripts are provided for more easily running jobs using many of the third party software packages. Most of these scripts are in the /apps/scripts directory and

have names starting with "run". For example, a Gaussian 16 job can be submitted to a queue by typing

```
run gaussian input_file_name
```

The queue script will prompt you for the name of the queue and any limits you may wish to set on time, memory or file size. It then prompts for a date and time to run the job, job name, and output directory. All prompts can be satisfied by pressing "Enter" to give default values of the queue limits, immediate submittal, a default job name, and results being returned to the current directory. Only class accounts can submit jobs to the class, class_uv, and class_gpu queues.

Accounts have a disk quota limit. To see your disk quota, type "quota". Queue limits and interactive use limits can be seen by typing "qlimits".

Please contact the Alabama Supercomputer Center staff if you have any other questions or concerns about using the supercomputers.

David Young, Ph.D.