

Getting Started with PENTRAN Tools

On **mc2** **AND** **aun** nodes:

In your `~/ .bash_profile`, append the following line

```
source /gpfs/lb/sets/cahrens/bash_profile
```

This will provide the tuned setting for using PENTRAN and related tools

General guidelines

On Ubuntu Linux terminal,

Log into bluem with '-Y' for X11 tunneling:

- `ssh -Y username@bluem`

Also, when logging into either 'mc2' or 'aun' (also allow tunneling):

- `ssh -Y mc2`

Things to know about the bluem cluster:

<http://hpc.mines.edu/bluem/description.html>

bluem consists of 2 partitions

1. mc2 - IBM Blue Gene Q - 512 nodes x 16 CPUs per node = 8,192 cores
 - a. 1GB per CPU
 - b. We will be running PENTRAN on the mc2 (BGQ) cluster
2. aun - iDataplex (intel) - 144 x 16 CPUs per node = 2,304 cores
 - a. 4GB per CPU
 - b. PENMSH needs to use aun because DISLIN graphics support is intel-based