Bob Documentation

- Bulletins
  - bulletins to see the list
  - bulletin $bulletin_name to read
- Computing Guide
  - Dated, but useful for getting started
- Wiki
  - More recent, but only covers some topics
- Man pages
- requests@cita.utoronto.ca

Environment Configuration

- Separate /home from CITA network!
- Shell Configuration
  - ~/.[ba,tc,c]shrc
  - setenv OMP_THREAD_NUM 2
  - unlimit, limit coredumpsize 0
- Modules
  - simple and dynamic env. configuration
  - module [list,avail,show $PACKAGE]
    - Define env. variables for makefiles, etc.
  - Put module load $PACKAGE statements in shell configuration to make them persistent
  - Available Packages:

    BLACS, GOTO, SCALAPACK, FFTW, HDF, Intel Compilers, Intel IPP, Intel MKL, LAM, OpenMPI, NetCDF, PGPlot
  - We'll install new packages on request

PBS (portable batch system)

- McKenzie uses TORQUE and Maui

Typical batch script (see bulletin for more examples):

```
#!/bin/csh
#PBS -l nodes=4:ppn=2
#PBS -q workq
#PBS -r n
#PBS -l walltime=06:00:00
cd $PBS_O_WORKDIR
lamboot
mpirun C myProgram < in >& out
lamhalt
```

- For reliable disk mounts:

```
#PBS -l other=raid-rjh:scratch-eh7:hoser1
```

- To use 2G nodes:

```
#PBS -l nodes=1:ppn=2:mem2g+nodes=1:ppn=2
```

- Do pre- and post-processing in your batch file:
  lamexec N $COMMAND

- short walltime duration jobs and jobs submitted by users who haven't run recently (2 week fairshare timescale) will move through the queue faster

Compilers and Debugging

Intel / Gnu compilers

- GCC has closed the performance gap and now supports threading with OpenMP
- -O3 for full optimizations, -O0 for none
- -[a]xN (intel only) processor specific optimization
- -g generate symbol table for debugging
- -CB / -fbounds-check (fortran only)
- -openmp / -fopenmp for OpenMP

Debugging

- Devel nodes – devel[1:4] for interactive use
- Debug on 1 node:
  - mpirun -np N xterm -e gdb a.out
- Larger jobs – print statements

Job Monitoring

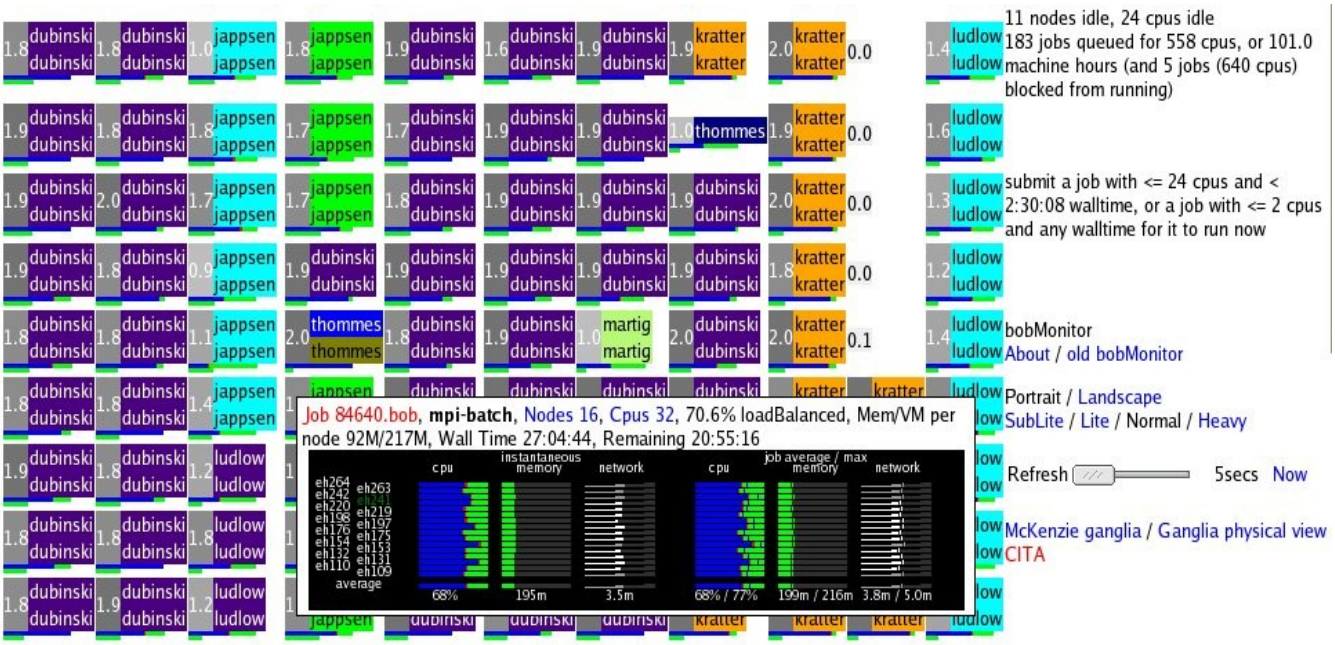
Command Line Utilities:

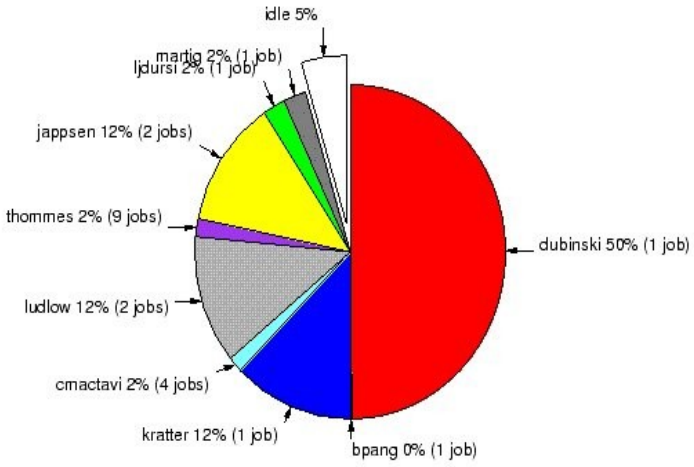
- qstat
  - -f $JOB_ID for detailed information about job
- showq
  - Resources requested and time queued
- freeNodes -A
  - Cluster summary
  - suggested quick runtime parameters

Web Based:

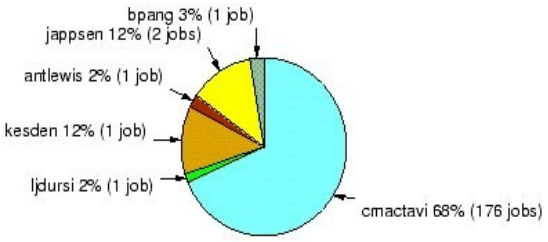
- bobMon
  - ssh -L 10101:bob:80 gw.cita.utoronto.ca
  - http://localhost:10101/bobMon
- More info at bobMon wiki page

BobMon





Running



Queued

PBS Job Output

- cita.pbs -> cita.e$JOB_ID & cita.o$JOB_ID
- Error files show any stderr output from your job
- Output files show:
  - Requested and Used Resources
    - Wall Time, Memory, Networking, Swapping
    - CPU States (user,sys,wait_io,idle)
    - Overall job efficiency
    - These contain network traffic and remote disk access overhead, so take with a grain of salt
  - Echo of the job script that was submitted