Computing Environment

Short Course on HPC

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Linux computing environment

- Linux OS
  - /
  - /home/username
- User environment
  - Terminal
  - Shell – Bash, csh, zsh...
  - Commands, paths
  - Environment Variables

SahasraT programming environment

- SahasraT is a Cray-XC40 system.
- Compilers, libraries etc required are set by **module load package**
- ex**. module load fftw**
- Default programming environment– Cray compiler **PrgEnv-cray**
- To change to GNU (similarly to intel)**,**
- **module swap PrgEnv-cray PrgEnv-gnu**
- Other commands
- **module list**
- **module avail**

HPC environment – Batch System

- Linux PC : Running program --> HPC cluster: Submit a job to resource manager
- Resource Manager
  - Operates queues
  - Starts, completes/kills jobs as per request/policy
  - Logs data
  - SahasraT resource manager – PBS Pro

  •IMPORTANT: SahasraT has lustre scratch file system. All jobs must have working directories in lustre, not in user home
- Job script examples

Job script

```
#!/bin/sh
#PBS -N jobname
#PBS -l select=10:ncpus=24 //select 10 compute nodes
#PBS -l walltime=24:00:00   //maximum walltime for a job to run
#PBS -l place=scatter
#PBS -l accelerator_type="None"
//add the above line only for idqueue,small,small72,medium queue
#PBS -S /bin/sh@sdb -V
. /opt/modules/default/init/sh

#(By default, PBS starts in $HOME. This step brings you back to directory of job submission)
cd $PBS_O_WORKDIR
#Launch the parallel job
aprun -j 1 -n 240 -N 24 ./name_of_executable
//Using 240 MPI processes and 24 MPI processes per node
```

SahasraT queue policy

- Queues
  - job streams, one job executed after another according to set policy.
  - Have per user and per queue run limits & submit limits
- Sahasrat queues

queue	Node (cores)	RunLimit User (queue)	Purpose, WaitTime
Idqueue	1-10 (1-240)	1 (32)	Debug, quick scheduling
Small	11 – 43 (240 – 1032)	3 (20)	Regular, several. ~1-2d
Small72	11-43	1 (11)	Reg, 72hr run &waitTime ~6d
medium	44 – 343 (1033 – 8208)	1 (12)	Reg, avg WaitTime. ~1d
large	344 – 1000 (8209 – 24000)	1 (1)	Reg big, long WaitTime. ~10d
Reservation	Any	1	Spl request. GuaranteedTime
Gpu, mgpu, knl			