Runing MPI jobs

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Open MPI 2.0.1 is currently installed in /share/apps on Prince. There are some notable differences between this version and those installed on Prince cluster:

- From the open-mpi.org web site:
  Please note that mpiexec/mpirun automatically binds processes as of the start of the v1.8 series. Two binding patterns are used in the absence of any further directives:
  - Bind to core - when the number of processes is \( \leq 2 \)
  - Bind to socket - when the number of processes is \( > 2 \)

- Slurm is plugged into this Open MPI installation as an environment-specific service. Open MPI automatically obtains directly from Slurm the list of hosts and the number of processes to start on each host. So it is unnecessary to specify the \(--hostfile, --host, or -np\) options to mpiexec/mpirun. Open MPI will also use SLURM-native mechanisms to launch and kill processes.

In the mpiexec PI calculation example below, it is expressed that this job requires 3 nodes, 4 tasks on each node, and 7 CPU cores for each task.
#!/bin/bash
#
#SBATCH --job-name=mpiexec-test
#SBATCH --nodes=3
#SBATCH --tasks-per-node=4
#SBATCH --cpus-per-task=7
#SBATCH --time=12:00:00
#SBATCH --mem=120GB

module purge
module load openmpi/intel/2.0.1

cd /share/apps/examples/mpi-openmp
mpiexec ./pi

After the job is submitted and running, check its status:

```bash
$ squeue -u $USER
  JOBID PARTITION     NAME     USER ST   TIME NODES NODELIST(REASON)
  6848    normal mpiexec-     wd35  R  0:07      3 c06-[01-03]
```

$ scontrol show job -dd 6848 # the command generates many line result including the following

```bash
NodeList=c06-[01-03]
BatchHost=c06-01
NumNodes=3 NumCPUs=84 NumTasks=12 CPUs/Task=7 ReqB:S:C:T=0:0:*:*
TRES=cpu=84,mem=360G,node=3
Socks/Node=* NtasksPerN:B:S:C=4:0:*:* CoreSpec=*
  Nodes=c06-[01-03] CPU_IDs=0-27 Mem=122880
```