Quick Summary
Center for Research Computing
University of Pittsburgh

Access
- Request an Account
  http://core.sam.pitt.edu/apply
- Login
  HTC ................................ htc.sam.pitt.edu
  SMP/OPA/NTA ............ h2p.crc.pitt.edu
- Storage
  ihome (75G per user) ............... /ihome
  mobydisk (2T per group) .......... /mnt/mobydisk
  ZFS (5T per group) ............... /zfs1 & /zfs2
  • your home directory on each of these storage systems is under your primary group name directory. It is backed up.
  • Use the id command to find your primary group.
  • Both mobydisk and ZFS are not backed up.
  • To get ZFS storage space open a help ticket.

Common Commands
- Connect
  ssh h2p.crc.pitt.edu #connect to the SMP, OPA and GPU clusters
  ssh htc.sam.pitt.edu #connect to the HTC cluster
- Data
  scp afile.tgz htc.sam.pitt.edu:~/ #copy from local computer to SMP cluster
  scp htcmob.smp.pitt.edu:/afile.tgz . #copy from htc to local computer
  rsync -aP $HOME/arc /zfs1/1/sam/ketan #copy src to zfs using rsync
  df -h /zfs1/2/kjordan/ #find quota of a group's ZFS storage
  lfs quota -g jpipas /mnt/mobydisk #find quota of a group’s mobydisk storage
- LMod: load and unload software
  module spider fftw #search for module named fftw
  module avail #list available modules
  module list #list currently loaded modules
  module load compiler/python/2.7.10-Anaconda-2.3.0 #load anaconda module
  module purge #unload all modules

Hardware
- SMP Standard 10 GIGE NETWORK
  • 100 nodes of 24-core Xeon Gold 6126 2.60 GHz (Skylake), 192 G RAM, 256 G & 500 G SSD
  • 24 nodes of 12-core Xeon E5-2643v4 3.40 GHz (Broadwell), 256 G RAM, 256 G SSD & 1 T SSD
- SMP Specialty
  • 2 nodes of 12-core Xeon E5-2643v4 3.40 GHz (Broadwell), 256 G RAM, 256 G SSD & 3 T SSD, 10 GigE
  • 2 nodes of 12-core Xeon E5-2643v4 3.40 GHz (Broadwell), 512 G RAM, 256 G SSD & 3 T SSD, FDR-IB
  • 1 node of 12-core Xeon E5-2643v4 3.40 GHz (Broadwell), 256 G RAM, 256 G SSD & 6 T NVMe, GigE
- OMNI-PATH NETWORK
  • 96 nodes of 28-core Intel Xeon E5-2690 2.60 GHz (Broadwell), 64 G RAM, 256 G SSD, 100 Gb
- INFINIBAND NETWORK
  • (IB) 32 nodes of 20-core Haswell (E5-2660 v3), 2.6 GHz (Haswell), 128 G RAM, 256 G SSD
- HTC INFINIBAND NETWORK
  • 4 nodes of 24-core Xeon Gold 6126 2.60 GHz (Skylake) 384 G RAM, 256 G & 500 G SSD
  • 20 nodes of 16-core Intel Xeon E5-2630v3, 2.4GHz (Haswell-EP), 256 G RAM, 256 G SSD
- NTA
  • 8 nodes of 256-core (hyper-threaded) Intel KNL Xeon Phi 7210 1.30 GHz, 94 G RAM
  • 7 nodes with 4 NVIDIA Titan X GPGPUs/node
  • 8 nodes with 4 NVIDIA GeForce GTX 1080 GPGPUs/node
  • 1 node with 2 NVIDIA K40 GPGPUs

Help
Does the FAQ answer your question?
http://core.sam.pitt.edu/faqs
Search the website:
http://core.sam.pitt.edu/search
Read the documentation
http://core.sam.pitt.edu/node/6
- When submitting support ticket
  1. Provide a descriptive, specific title
  2. Specify the cluster the ticket applies to
  3. Provide directory location if applicable

- CRC Consultants and their Expertise
  Kim Wong: Bio Simulation | Agent-based Modeling | Physics-based Modeling
  Fangping Mu: Bioinformatics | Computational Biology | Computational Genomics
  Barry Moore: Quantum Chemistry | HPC
  Ketan Maheshwari: GPU Computing | Scientific Workflows
  Sherwin Sammak: Turbulent Combustion | Fluid Dynamics

- Contact / Feedback
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Job Scheduler Policy
Details coming soon.
- Charging
  Users are charged in terms of Service Units (SU) which depend on both memory and CPU usage.
- Queues and limits
  - Minimum and maximum walltimes
  - Minimum and maximum nodes that may be requested

Software
- Applications
  • Chemistry: NAMD®, casino, lammps, Amber®, Molpro®, Turbomole®, CP2K®, Gaussian®
  • Bio: CLCbio®, galaxy®, bowtie®, samtools®, picard®, trinity®
  • Material Sci: Material Studio, Westpa, abaqus, VASP®
- Libraries and Programming
  • Compilers: GCC®, Python®️, Perl®, R®, Matlab
  • Libraries: Boost®, FFT®, tensorflow®, mkl®, hdf5®, biocoordinator®️
- Others
  • Editors: vim®, emacs®, nano®, gedit®,
  • Debuggers: gdb®, gprof®,
  • Shells: bash®, zsh®️

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  • Bio: CLCbio®, galaxy®, bowtie®, samtools®, picard®, trinity®
  • Material Sci: Material Studio, Westpa, abaqus, VASP®
- Libraries and Programming
  • Compilers: GCC®, Python®, Perl®, R®, Matlab
  • Libraries: Boost®, FFT®, tensorflow®, mkl®, hdf5®, biocoordinator®️
- Others
  • Editors: vim®, emacs®, nano®, gedit®,
  • Debuggers: gdb®, gprof®,
  • Shells: bash®, zsh®️
### Quick Summary

**Center for Research Computing University of Pittsburgh**

#### Computation

CRC clusters use the SLURM scheduler.

- **Job Management**
  - `sinfo` #view info about nodes
  - `sbatch` job #submit a job
  - `squeue` #check job status
  - `scancel` job id #cancel job with id

Below is the command to see details of the nodes on a particular cluster. The key column is the CPUS(A/I/O/T) where, A = allocated, I = idle, O = other, T = total

Single-core jobs should fit within nodes with non-zero I.

- **Note:** The above commands will show info about the SMP cluster by default. To see info about other clusters, use the --cluster option with name of cluster, eg. `squeue --cluster=hpc`

- **example**
  - `h2p.crc.pitt.edu`

- **Example SLURM Scripts**

**- for HTC**

```bash
#!/bin/bash
#SBATCH --job-name=testR
#SBATCH --nodes=2
#SBATCH --ntasks=1
#SBATCH --time=00:10:00
#SBATCH --output=gputf.std.out
#SBATCH --reservation=sam_4
#SBATCH --qos=long # required if walltime is greater than 3 days
#SBATCH --mail-type=END,FAIL # ... job ends or fails
#SBATCH --mail-user=shs159@pitt.edu #send email to this address if ...
#SBATCH --cluster=mpi # cluster name is required
#SBATCH --partition=opa # partition name is required
#SBATCH --ntasks-per-node=1
#SBATCH --nodes=2 #number of nodes requested
#!/bin/bash
export I_MPI_FABRICS_LIST=tmi:I_MPI_FALLBACK=0
```

**- for SMP/MI/P/OPA**

```bash
#!/bin/bash
#SBATCH --job-name=testR
#SBATCH --nodes=2
#SBATCH --ntasks=1
#SBATCH --time=00:10:00
#SBATCH --output=test.out
#SBATCH --job-name=testR #name of job: will show up in status output of
#SBATCH -t 00:10:00 # 10 minutes walltime in HH:MM:SS format
#SBATCH --error=test.err
```

**- for GPU**

```bash
#!/bin/bash
#SBATCH --job-name=gputf
#SBATCH --output=gputf.std.out
#SBATCH --error=gputf.std.err
#SBATCH --time=00:10:00
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cluster=gpu
#SBATCH --partition=gp
#SBATCH --gres=gpu:4
```

### Troubleshoot

- **SSH connection**
  - If you are on a wireless network, make sure the VPN connection is established.
  - Use `ping` to check network connectivity to host, eg. `ping htc.sam.pitt.edu`
  - Use `ssh` in verbose mode with `-v` to identify possible causes, eg. `ssh -v h2p.crc.pitt.edu`

- **Jobs submission**
  - Sanity test the environment by submitting a simple job, eg. `#!/bin/bash
  
  #SBATCH --output=test.out
  
  #SBATCH --error=test.err
  
  #SBATCH --time=00:10:00
  
  #SBATCH --output=test.out
  
  #SBATCH --error=test.err`

- **Software access**
  - Check if the software is available using `module list`
  - Check if the module is loaded with `module avail`

- **Notes**
  - In software, superscripts indicate availability over a cluster: h=HTC, s=SMP, g=GPU, o=OPA, items in red indicate licensed software
  - To print this document on letter size paper use the printer’s `fit to size` option.
  - `BiGxi` source on git: `github.com/ ketancmaheshwari/crc_cheatsheet`

- **Acronyms**

  | HTC       | High Throughput Computing       |
  | SMF       | Shared Memory Processing       |
  | OPA       | Omni-Path                     |
  | IB FDR    | InfiniBand Fourteen Data Rate  |
  | GPV       | Graphics Processing Unit      |
  | SSD       | Solid State Drive             |
  | NTA       | Non-Traditional Architecture   |
  | NVMe      | Non-volatile Memory express    |
  | ZFS       | Zettabyte File System         |