

# QUICK SUMMARY

## CENTER FOR RESEARCH COMPUTING

### UNIVERSITY OF PITTSBURGH

#### Useful Links

- H2P Documentation: <https://crc.pitt.edu/h2p>
- HTC Documentation: <https://crc.pitt.edu/htc>
- Submit a Ticket: <https://crc.pitt.edu/tickets>
- CRC Status: <https://crc.pitt.edu/status>
- Proposals, Renewals, and Allocations: <https://crc.pitt.edu/apply>
- Hardware Description: <https://crc.pitt.edu/Resource-Description-Proposal-Language>
- Submit Citations: <https://crc.pitt.edu/doi>
- Submit Feedback: <https://crc.pitt.edu/contact>

#### Access Environments

- **Connect to the VPN when off-campus or on Pitt WiFi!**
  - Details: <https://crc.pitt.edu/h2p#Off-campus-access>
- Login Nodes: `h2p.crc.pitt.edu` or `htc.crc.pitt.edu`
- Jupyter Notebooks: <https://hub.crc.pitt.edu>
- Visualization: <https://viz.crc.pitt.edu>
- Open OnDemand: <https://ondemand.htc.crc.pitt.edu>
- Galaxy: <https://crc.pitt.edu/galaxy>
- CLC Genomics: <https://crc.pitt.edu/clcbioserver>

#### Storage

- Mount points and quotas:
  - Iscsi (75G per user) `/ihome`
  - ZFS (5TB per group) `/zfs1` or `/zfs2`
  - BGFS (5TB per group) `/bgfs`
- Policies:
  - Your home directory will be located in `/ihome` and is backed up

- BGFS and ZFS are **not** backed up
- Each group can have up to 5TB on BGFS or ZFS for free
- To get access to BGFS or ZFS submit a ticket

#### Useful Commands

- Connect via secure shell `ssh <username>@h2p.crc.pitt.edu`
- Transferring data:
  - `scp <file> <username>@h2p.crc.pitt.edu:~`  
*## local to remote*
  - `scp <username>@h2p.crc.pitt.edu:~/<file> .`  
*## remote to local*
- Check your filesystem quotas: `crc-quota.py`
- Check your service units quotas: `crc-usage.pl`

#### Software

- Search all available software: `module spider`  
*## Use '/' for search, 'q' quits*
- Load a module: `module load <module>`
- List loaded modules: `module list`
- Purge your modules: `module purge`

#### Getting Help

- When submitting a support ticket:
  - Use a descriptive and specific title
    - \* Bad: Command doesn't work
    - \* Good: Gaussian is failing with <abbreviated error here>
  - Provide enough information for us to reproduce your problem, e.g.
    - \* The input and output file with exact paths
- CRC Consultants with Expertise
  - Kim Wong: Molecular Dynamics | Agent-based Modeling
  - Fangping Mu: Bioinformatics | Computational Biology/Genomics
  - Barry Moore II: Computational Chemistry | Deep Learning
  - Shervin Sammak: Computational Fluid Dynamics
  - Leonardo Bernasconi: Computational Chemistry
- Comments and suggestions for improvement can be submitted at <https://crc.pitt.edu/contact>

#### Slurm Jobs

- Show your jobs only: `crc-squeue.py`
- Cancel a job: `crc-scancel.py <jobid>`
- Submit an interactive job: `crc-interactive.py -s`
- Submit a batch job: `sbatch <file>`
- Browse clusters and partitions: `crc-squeue.py`
- Add this to the end of your batch scripts: `crc-job-stats.py`
- Example job scripts, browse `/ihome/crc/how_to_run`
- Description of `sbatch` arguments:
  - `job-name`: This name shows up in `crc-squeue.py`
  - `output`: Standard input/output will be written to this file
  - `time`: How long your job will run for  
(format: `[days-]hours:minutes:seconds`)
  - `nodes`: How many nodes your job needs
  - `ntasks-per-node`: How many MPI processes your job needs per node, pro tip: if you don't know what this means it should be equal to 1
  - `cpus-per-task`: Either the number of cores or OpenMP threads
  - `cluster`: Run on this cluster, try `crc-sinfo.py` to see clusters
  - `partition`: Run on this partition, try `crc-sinfo.py` to see partitions
  - `mail-user`: Set to your Pitt email address to get updates (optional), pair with `--mail-type=END,FAIL`
- Reasons from `crc-squeue.py` (don't submit a ticket unless specified)
  - `Priority`: You are waiting in line
  - `MaxCPUPerAccount`: You are waiting in line because your group is running on too many cores
  - `MaxMemoryPerAccount`: You are waiting in line because your group is using too much memory
  - `GrpTresRunMinsLimit`: Your group is out of service units. Submit a ticket!

#### Notes

- Is something not working? <https://crc.pitt.edu/tickets>
- Suggestion or improvement for this document: <https://github.com/barrymoo/crc-quicksummary/issues/new>