

The CBCB computational infrastructure

Computer resources

- Desktop machines
 - note: slow network connection to UMIACS servers
- High memory 'servers'
 - 3 (soon 4) 64-core, 512 GB RAM, 2 TB disk servers
 - several older (and soon defunct) servers
- Cluster(s)
 - condor – ibis cluster (~250 cores)
- All machines available through torque (soon through Slurm?)

<https://wiki.umiacs.umd.edu/cbcb-private/index.php/Compute>

Torque usage (brief)

- <https://wiki.umiacs.umd.edu/cbcb/index.php/Torque>
- CBCB queues
 - shell – interactive shell
 - throughput – many jobs with limited resources (<4GB)
 - long – long running job (up to 1 week)
 - large – high memory, long running
 - xlarge – even higher memory and time limits [restricted]
- Basic protocol
 - create shell script containing job (and requirements)
 - submit script through 'qsub' command

Torque to Slurm

- System will be transitioned to Slurm – de facto standard for HPC infrastructures (deephought2, XSEDE, etc.)
- See <http://slurm.schedmd.com/tutorials.html>
- Not much will change (other than syntax)
 - e.g. 'qsub' becomes 'sbatch'

Non-CBCB resources

- UMIACS
 - UMIACS condor pool (includes CBCB machines)
 - new UMIACS Amazon-like service
 - Jimmy Lin cluster (just funded – will require negotiation for access)
- Campus
 - deepthought1/deepthought2 – allocations may be available through department/college
 - CMNS condor pool (fairly small)
- External
 - AWS (\$\$)
 - XSEDE and other public HPC infrastructures (require proposal to obtain allocations)
- Special:
 - Lattice project, BOINC, Garli, etc. - already support phylogenetic analyses and special applications of broad interest could be supported – needs coord. with Cummings lab and code devel.

Computer usage policies

- pay attention to usage before starting job
- stage data to local disk (/scratch0, /scratch1)
- concurrent accesses from 100+ machines will kill our file server
- clean up after yourselves (don't leave stuff in /scratch*)
- it is not OK to submit thousands of jobs

Disk space

Lab specific, backed up, little space

/cbcb/lab/<pi_name>

(e.g., /cbcb/lab/hcorrada)

Shared scratch/not backed up, lots of space

/cbcb/personal-scratch – for personal stuff, local sandboxes, etc.

/cbcb/project-scratch – for specific projects

/cbcb/project2-scratch

Local scratch

available on each machine (not centrally mounted)

/scratch

Usage policies

- currently self-policing
- other centers – files automatically deleted 30 days past creation

Disk policies

- Clean up old data
- Check in on long-running programs and disk usage
- Stage critical data to backed up space

- Clinical data – treat carefully.

Printers/policies

- Room number in printer name
- e.g. ps-296-3120H – main Xerox printer in 3120H
- cps-296-3120Hb – color printer in 3120H
- suffix 'nb' means 'no banner page'

- No printing of personal material
- No copyright infringement
- Retrieve your print jobs promptly
- Daily pile in room 3120H – piles recycled weekly

<https://wiki.umiacs.umd.edu/umiacs/index.php/Printing>

Software resources

- /cbcb/software
 - anyone can install software
- /cbcb/core-software/
 - important core software
- /cbcb/data
 - common useful datasets (e.g., NCBI database dumps, bowtie indices, etc.)
- **DO NOT CONTACT staff@umiacs FOR SOFTWARE ISSUES!**
- ...until you learn from other CBCB folks that it's an IT issue

Modules

- Software environment managed through 'modules'
- Include CBCB-specific configuration in your:
 - `.bashrc` :
 - `./cbbc/software/share/dotfiles/bashrc.cbbc`
 - `.tcshrc` :
 - `source /cbbc/software/share/dotfiles/tcshrc.cbbc`
- Find out about available modules
 - `module avail`
- Select a specific configuration
 - `module load Python`
 - `module load Python/2.7.8`
- Create your own module files
 - environment variable `MODULEPATH`
 - `man modulefile`

Website

Old school home pages

- /fs/www/users/<username>
- <http://www.cbcb.umd.edu/~<username>>

Drupal

- Logging on:
 - <http://www.cbcb.umd.edu/user>
- Modifying your profile [please do even if you have a page]
 - <http://www.cbcb.umd.edu/people/<username>>
- Adding publications
- Creating content

Please send suggestions for improvement to us!

Others

- Resources/information
 - wiki.umiacs.umd.edu
 - wiki.umiacs.umd.edu/cbcb
 - wiki.umiacs.umd.edu/cbcb-private
- Bi-weekly maintenance
 - all computers down
- staff@umiacs.umd.edu
 - help with general infrastructure
 - no help with bioinformatics-specific stuff
- The CBCB 'elders'
 - that way you also get to meet other members of the Center