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)

- 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 (deepthought2, 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

https://wiki.umiacs.umd.edu/cbcb-private/index.php/Storage
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:
    . /cbcb/software/share/dotfiles/bashrc.cbcb
  – .tcshrc:
    source /cbcb/software/share/dotfiles/tcshrc.cbcb
• 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/cbc
  - wiki.umiacs.umd.edu/cbc-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